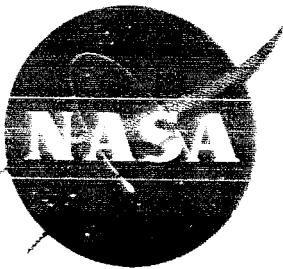


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FACILITY FORM 602

**INVESTIGATION OF
NONEQUILIBRIUM FLOW EFFECTS
IN HIGH EXPANSION RATIO NOZZLES**

COMPUTER PROGRAM MANUAL

by

T.F. ZUPNIK, E.N. NILSON, and V.J. SARLI

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| CATEGORY | |

prepared for

NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

CONTRACT NAS 3-2572

CTS PRICE

KEROX \$ 3.67
MICROFILM \$ 25

Research Laboratories

U
UNITED AIRCRAFT CORPORATION
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EAST HARTFORD, CONNECTICUT

ERRATA dated 2/19/73 imported

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NASA CR-54042
UACRL C-910096-11

TOPICAL REPORT

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NATIONAL AERONAUTICS AND SPACE ADMINISTRATION

September 15, 1964

CONTRACT NAS3-2572

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Cleveland, Ohio
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East Hartford, Connecticut

INVESTIGATION OF NONEQUILIBRIUM FLOW EFFECTS IN
HIGH EXPANSION RATIO NOZZLES

Computer Program Manual

TABLE OF CONTENTS

| | <u>Page</u> |
|---|-------------|
| ABSTRACT | i |
| FOREWORD | ii |
| SUMMARY | 1 |
| INTRODUCTION | 1 |
| DESCRIPTION OF ANALYSIS | 4 |
| Modes of Operation | 4 |
| <u>Combustion Chamber</u> | 4 |
| <u>Nozzle</u> | 4 |
| Equation System | 4 |
| <u>Assumptions</u> | 4 |
| <u>The Gas Dynamic Equations</u> | 5 |
| <u>The Reaction Kinetics Equations</u> | 7 |
| Numerical Techniques | 8 |
| <u>Modified Equation System</u> | 8 |
| <u>Integration Routine</u> | 10 |
| <u>Round-Off Error Control</u> | 13 |
| <u>Integration in the Transonic Region - Throat Control</u> | 13 |
| <u>Throat Study</u> | 14 |
| DISCUSSION OF THE MACHINE PROGRAM | 15 |
| Input Description | 15 |

TABLE OF CONTENTS
(Cont.)

| | <u>Page</u> |
|---|-------------|
| <u>Input Listing</u> | 15 |
| <u>Sample Input</u> | 19 |
| | |
| Output Description | 20 |
| Common Operational Problems | 21 |
| | |
| <u>Selection of Starting Location</u> | 21 |
| <u>Choice of Critical Mass Flow Rate</u> | 21 |
| <u>Aborted Starting</u> | 22 |
| <u>Machine Overflow</u> | 22 |
| | |
| REFERENCES | 23 |
| | |
| LIST OF SYMBOLS | 24 |
| | |
| APPENDIX I - LISTING OF SUBROUTINES AND FLOW CHARTS | 26 |
| | |
| APPENDIX II - DISTRIBUTION LIST | 43 |
| | |
| TABLES | 52 |
| | |
| FIGURES | 63 |

ABSTRACT

Investigation of Nonequilibrium Flow Effects in
High Expansion Ratio Nozzles
Computer Program Manual

by

T. F. Zupnik, E. N. Nilson, and V. J. Sarli

31452

A machine computational program developed by the United Aircraft Corporation to treat the one-dimensional flow of reacting gas mixtures in variable area passages has been modified as part of NASA Contract NAS3-2572 to facilitate general use of the program on the NASA Lewis Research Center IBM 7094 Computer. This machine computational program numerically integrates the system of reaction-kinetic, gas-dynamic and state equations to calculate compositions and thermodynamic properties in both subsonic and supersonic flow passages.

This report describes the equations and numerical techniques employed and presents flow charts and specific instructions for input formats and operation of the machine program.

Also included is a discussion of possible operational problems which might arise prior to complete familiarization with the program together with appropriate means for solving these problems and avoiding their recurrence.



FOREWORD

This work was performed by United Aircraft Corporation Research Laboratories for the National Aeronautics and Space Administration under Task V of Contract NAS3-2572 initiated September 4, 1963. This task involved conversion and modification of a computer program originally developed by the UAC for treating one-dimensional gas dynamic flows with finite reaction kinetics in order to provide the NASA with a copy of the computer deck suitable for general use on the IBM 7094 machine.

Included among those who cooperated in performance of the work under Contract NAS3-2572 were Dr. V. J. Sarli, Program Manager; Mr. A. W. Blackman, Chief, Rocket and Air-Breathing Propulsion Section; and Dr. W. G. Burwell, Supervisor, Kinetics and Heat Transfer Group of the UACRL and Dr. E. N. Nilson, Chief, Scientific Staff and Mr. T. F. Zupnik, Scientific Staff of Pratt & Whitney Aircraft Division of UAC.

This work was conducted under the program management of Mr. H. Burlage, Jr., Chief, Liquid Propulsion Systems, NASA Headquarters, Washington, D. C. and the Project Manager was Mr. P. N. Herr, NASA Lewis Research Center, Cleveland, Ohio.

This document is unclassified in its entirety.

INVESTIGATION OF NONEQUILIBRIUM FLOW EFFECTS IN
HIGH EXPANSION RATIO NOZZLES

Computer Program Manual

T. F. Zupnik, E. N. Nilson and V. J. Sarli

United Aircraft Corporation

SUMMARY

A description is contained herein of a machine computational program developed to calculate the nonequilibrium flow properties of chemically reacting gas mixtures in one-dimensional flow fields. This program is applicable in subsonic, transonic, and supersonic flow regimes such as are found in the combustion chamber and expansion nozzle of a liquid rocket or ramjet engine. The calculations performed using this program may be initiated directly from a state of thermodynamic equilibrium. Also, the chemical kinetic relationships can be treated without loss of accuracy as near-equilibrium conditions are approached.

Extensive flow charts, input and output formats and general instructions for the use of the program are included in this manual. The input instructions are illustrated for a typical calculation using the chemical kinetic scheme pertinent to the hydrogen-oxygen propellant combination.

INTRODUCTION

The design of rocket exhaust nozzles to provide maximum expansion efficiency requires accurate methods for evaluating nonequilibrium flow processes and the effects of nozzle contour and size on such processes. The nonequilibrium processes which are of significance (depending on the propellant combination and operating conditions) include chemical recombination lags, thermodynamic relaxation lags, condensation lags and velocity and thermal lags associated with two phase flow. United Aircraft Research Laboratories has been selected under Contract (NASw-366 and NAS3-2572) to investigate the nonequilibrium flow processes in high expansion ratio nozzles and to develop improved techniques for predicting the performance of rockets utilizing high energy propellants. The nonequilibrium processes were in-

vestigated for a variety of propellant combinations and it was confirmed (Ref. 1) that nonequilibrium chemistry would be a significant factor in limiting the theoretical performance of all the propellants considered at typical rocket conditions.

Three machine computational programs have been developed in connection with these contracts to treat nonequilibrium flows of reacting gas mixtures in both one-dimensional and two-dimensional or axisymmetric exhaust nozzles. The one-dimensional flow computer program is described in detail in this report and both the one-dimensional and two-dimensional or axisymmetric flow programs are described generally in Ref. 1. The machine programs for constructing two-dimensional or axisymmetric flows with finite chemical kinetics consist of a "performance deck" which can be used to evaluate the performance of a prescribed nozzle contour, and a "design deck" which can be used in the determination of an optimum nozzle contour. The studies reported under Contract NASW-366 demonstrate that the one-dimensional and two-dimensional machine computation programs for reactive gas flows can predict experimental measurements of nozzle flow properties when the kinetics of the reactions occurring in the system are known.

Contract NAS3-2572 is currently in progress and involves the application of the machine computation programs to investigate selected problems associated with chemical nonequilibrium nozzle flows. These problems include sensitivity of performance to reaction rates, nozzle geometry and nozzle scale. While these studies have not been completed, preliminary results have been reported in Refs. 2, 3, and 4 and the final results of these studies will be reported in a Final Report late in 1964.

Modification of the one-dimensional finite-kinetics machine program to facilitate its use on the NASA Lewis Research Center IBM 7094 Computer was a requirement of Contract NAS3-2572. Wide interest in this program and increased demand for the needs of nozzle reactive-flow performance calculations has warranted the publication of a separate report describing this machine program. The objective of the material presented herein is to fulfill this need. The subsequent pages of this report present the equations and derivation of the equations for one-dimensional reactive gas flow systems in forms suitable for numerical computations. A set of equations transformed to facilitate calculations for near-equilibrium flow and in the transonic region of convergent-divergent nozzles is also included. In addition, a description of the numerical techniques and the integration routines is presented along with a discussion of round-off-error control.

Extensive flow charts are included which should permit a computer specialist to alter the machine program and tailor the numerical techniques for specialized systems if such alterations are desirable.

Information such as input and output formats, instructions for performance calculations involving various combustion chamber and nozzle combinations, and preselected nozzle throat contours are included. A sample calculation is presented for the recombination of the combustion products of H₂-O₂ in a convergent-divergent nozzle involving a multireaction system.

This program has been developed for and checked out on the standard IBM 7094 computer; however, due to possible variations among different monitoring systems employed at the various 7094 installations, a zero divide card or other minor modifications may be required in order to achieve satisfactory operation. For this reason NASA and UAC cannot guarantee successful program execution during the initial run. For the above mentioned reasons neither of the previously mentioned organizations shall be contacted concerning operational difficulties until all possible in-house computer and programming capabilities have been exhausted. In the event a major problem still remains unresolved, the NASA-Lewis Research Center should be consulted.

The one-dimensional nonequilibrium-flow kinetic program may be obtained by contacting IBM Program Distribution Center, P. O. Box 790, White Plains, New York (10601).

DESCRIPTION OF ANALYSIS

Modes of Operation

The machine procedure developed for analysis of one-dimensional chemically-reacting flows numerically integrates the system of reaction kinetic, gas dynamic and state equations to calculate bulk thermodynamic properties and chemical composition in both subsonic and supersonic flow passages of varying cross-sectional area. There is a considerable amount of flexibility in the deck which may operate in either of two modes; (1) combustion chamber, or (2) nozzle. The equation system and numerical techniques are basically the same in both modes but there are differences in the controls and input information necessary for each mode.

Combustion Chamber

In a combustion chamber it is assumed that the oxidant and fuel are individually in equilibrium and are then instantaneously mixed at an arbitrarily selected temperature. The resulting mixture is homogeneous but not in chemical equilibrium. The numerical integration proceeds from this point of mixing. The combustion chamber contour can be of the general form $A = ax + b$ where A is the cross section area at any axial location x, b is the initial area and a is the slope. The flow in the chamber may be either subsonic or supersonic. Starting from given conditions of temperature, pressure, velocity and composition, the numerical integration continues until one of three criteria is met. In subsonic combustion if the length of the chamber exceeds the maximum desired length or the temperature gradient falls below a prescribed tolerance, the calculation will stop, while in supersonic flow in addition to these, the calculation will be terminated when the difference between the Mach number and unity is less than a prescribed amount.

Nozzle

A nozzle contour may be prescribed by any area distribution which is input in tabular form and subsequently spline-fitted. The starting point of the calculation may be anywhere in the nozzle where the temperature, pressure, velocity and composition are known. The numerical integration proceeds using the given area distribution until the transonic region, described below, is reached or until either a preselected Mach number or nozzle length is exceeded.

Equation System

Assumptions

The basic assumptions in the formulation of the physical model of the flow

of a reacting gas mixture in a one-dimensional passage are:

- a. The mixture is one of thermally perfect gases.
- b. The flow is inviscid throughout.
- c. Transport properties can be neglected.
- d. The internal energies are those pertaining to thermal equilibrium.
- e. The law of mass action applies throughout.

The Gas Dynamic Equations

Total mass conservation:

$$\rho V A = \dot{m} \quad (1)$$

Total energy conservation:

$$H + \frac{V^2}{2g_j} = H_0 \quad (2)$$

where

$$H = \sum_{i=1}^n h_i \sigma_i \quad *(2a)$$

and where

$$h_i = \int_{T_b}^T C_{P_i} dT + (H_{f_i})_b \quad (2b)$$

Momentum conservation:

$$VV' + \frac{g}{\rho} P' = 0 \quad **(3)$$

* Unless otherwise noted, all summations are from $i = 1, \dots, n$.

** Prime values are derivatives with respect to X unless otherwise noted.

Equation of state:

$$P = \rho R T \Sigma \sigma \quad (4)$$

Speed of sound:

$$C = \sqrt{g \left(\frac{\partial P}{\partial \rho} \right)_{s, \sigma_1, \dots, \sigma_n}} = \sqrt{g \gamma R T \Sigma \sigma_i} \quad (5)$$

where γ is defined as:

$$\gamma = \frac{J \sum C_{P_i} \sigma_i}{J \sum C_{P_i} \sigma_i - R \sum \sigma_i} \quad (5a)$$

Mach number:

$$M = \frac{V}{C} \quad (6)$$

The above equations are operated upon and rearranged to provide the final set of equations which are numerically integrated in the machine program.

Differentiating Eq. (4) and eliminating P' from Eq. (3)

$$VV' + \frac{g}{\rho} \left[\rho' R T \Sigma \sigma_i + \rho R T' \Sigma \sigma_i + \rho R T \Sigma \sigma_i' \right] = 0 \quad (7)$$

Differentiating Eq. (2) and from Eqs. (3) and (4)

$$g J \left[\Sigma h_i \sigma_i + T' \Sigma C_{P_i} \sigma_i \right] + VV' = 0 \quad (8)$$

Combining Eqs. (6) and (7) and solving for

$$\frac{\rho'}{\rho} = \frac{T'}{T} \left(\frac{1}{\gamma-1} \right) - \frac{\Sigma \sigma_i'}{\Sigma \sigma_i} + \frac{J \Sigma h_i \sigma_i'}{R T \Sigma \sigma_i} \quad (9)$$

Differentiating Eq. (1) and eliminating $\frac{\rho'}{\rho}$ from Eq. (9) and combining with Eq. (8) to eliminate V' ,

$$T' = \frac{\frac{A'}{A} - \frac{\sum \sigma_i'}{\sum \sigma_i} + J \sum \sigma_i' h_i \left(\frac{1}{RT \sum \sigma_i} - \frac{g}{V^2} \right)}{J \sum C_{P_i} \sigma_i \left(\frac{g}{V^2} - \frac{1}{RT \sum \sigma_i} \right) + \frac{1}{T}} \quad (10)$$

combining Eqs. (10), (6), (2) and (5a)

$$T' = \frac{2(H_0 - H) \left(\frac{A'}{A} - \frac{\sum \sigma_i'}{\sum \sigma_i} \right) + \left(\frac{2(H_0 - H)}{T \sum \sigma_i C_{P_i}} + M^2 - 1 \right) \sum h_i \sigma_i'}{(1 - M)^2 \sum C_{P_i} \sigma_i} \quad (11)$$

The Reaction Kinetics Equations

Let n_r designate the total number of chemical reactions of the form:



where: a_{ij}', a_{ij}'' are the stoichiometric coefficients of the i th species in the j th reaction ($j = 1, 2, \dots, n_r$), reactants and products, respectively.

K_{fj}, K_{bj} are the specific reaction rates of the forward and backward chemical changes in the j th reaction of the chemical system.

The rates of change of the concentrations of the species M_i are determined by the relation

$$\frac{\partial [M_i]}{\partial t} = \sum_{j=1}^{n_r} (a_{ij}'' - a_{ij}') \left\{ K_{fj} \prod_{k=1}^n [M_k]^{a_{kj}'} - K_{bj} \prod_{k=1}^n [M_k]^{a_{kj}''} \right\} \quad (13)$$

where n designates the total number of chemical species such as M_1 of which n_a are the atomic species and $n-n_a$ are the number of molecular species, n_m .

Of the n_r chemical reactions, the first n_m are required to be independent (see sample input in a subsequent section of this manual), i.e., the matrix

$$\left\{ \begin{array}{l} a''_{n_a+1,1} - a'_{n_a+1,1}, \dots, a''_{n,n} - a'_{n,n} \\ a''_{n_a+1,2} - a'_{n_a+1,2}, \dots, a''_{n,2} - a'_{n,2} \\ a''_{n_a+1,n_m} - a'_{n_a+1,n_m}, \dots, a''_{n,n_m} - a'_{n,n_m} \end{array} \right\} \quad (14)$$

is nonsingular. The remaining sets of stoichiometric coefficient differences may be expressed as linear combinations of these sets. The atomic species continuity equations are given by:

$$\sigma_i + \sum_{j=n_a+1}^n \beta_{ij} \sigma_j = \text{constant} \quad (i=1,2,\dots,n_a) \quad (15)$$

where β_{ij} is the number of the i th atomic species in the j th molecular species. The molecular species continuity equations are thus given by:

$$\rho v \sigma'_i = \sum_{j=1}^{n_r} (a''_{ij} - a'_{ij}) \left[K_{f,j} \prod_{k=1}^n (\rho \sigma_k)^{a'_{kj}} - K_{b,j} \prod_{k=1}^n (\rho \sigma_k)^{a''_{kj}} \right] \quad (i = n_a+1, n_a+2, \dots, n) \quad (16)$$

Equations (1), (2), (4), (11), (15) and (16) along with an area function can be integrated to specify completely the flow. There are, however, certain numerical difficulties associated with the integration of this system which are discussed below.

Numerical Techniques

Modified Equation System

Two major difficulties exist in integrating the above system of equations

through a convergent-divergent nozzle that is flowing choked. These arise from (a) the necessity of integrating the equation through the sonic location, and (b) the significant figure loss when the flow is near equilibrium.

The first difficulty results from a singularity in the flow equation which occurs at $M = 1$ (see Eq. (11)). In order for the temperature gradient to remain negative throughout the nozzle, the numerator of the right hand side of Eq. (11) must pass through zero at the same time as the denominator does (at the sonic point). In general the location of the sonic point cannot be determined "a priori", and if the calculation is allowed to proceed at will, either the nozzle will not choke or will not be able to contain the flow. In order to handle this problem directly on the machine, a second set of equations is used in the transonic region. Equation (2) can be written

$$2gJ(H_0 - H) = M^2 \gamma g RT \sum \sigma_i \quad (17)$$

Differentiating this, and using (2a) and (2b), gives

$$T' = \frac{- \left(\frac{\sum h_i \sigma'_i}{H_0 - H} + \frac{2M'}{M} + \frac{\gamma \sum \sigma'_i}{\sum \sigma_i} - (\gamma - 1) \frac{\sum c_{p_i} \sigma'_i}{c_{p_i} \sigma_i} \right)}{\frac{1}{T} - (\gamma - 1) \frac{\sum \frac{dc_{p_i}}{dt} \sigma_i}{\sum c_{p_i} \sigma_i} + \frac{2}{\gamma - 1} - \frac{1}{TM^2}} \quad (18)$$

By specifying the Mach number distribution through the transonic region and using Eqs. (1), (2), (4), (15), (16) and (18) the singularity problem is averted and a method for multi-throat design is incorporated into the procedure.

The second difficulty which relates to the loss of significant figures in the numerical integration is given in Eq. (16). This equation introduces the possibility of accumulating serious error in all flow properties when any reaction is nearly in equilibrium. In particular, the factor

$$K_{fj} \prod_{k=1}^n (\rho \sigma_k)^{a'_k} - K_{bj} \prod_{k=1}^n (\rho \sigma_k)^{a''_k}$$

will involve the difference of two quantities of large size whose difference is very small. To avoid this loss in significant figures and to permit the initiation of the integration at equilibrium if desired, the variables λ_j are

introduced, where

$$\lambda_j = K_{Cj} \prod_{i=1}^n (\rho \sigma_k)^{\alpha'_{kj} - \alpha''_{kj}} - 1 \quad j = 1, 2, \dots, n_r \quad (19)$$

and $K_{Cj} = \frac{K_{fj}}{K_{bj}}$ is the equilibrium constant for the j th reaction. The quantities λ_j , associated with the reactions are now introduced as dependent variables replacing the quantities σ_j , associated with molecular species.

The differential equations (Eq. (16)) for the molecular species continuity are replaced by

$$\frac{\lambda'_j}{1 + \lambda_j} = \frac{\rho'}{\rho} \sum_{i=1}^n (\alpha'_{ij} - \alpha''_{ij}) + \sum_{i=1}^n (\alpha'_{ij} - \alpha''_{ij}) \frac{\sigma'_i}{\sigma_i} + \frac{1}{K_{Cj}} \frac{dK_{Cj}}{dT} T' \quad (20)$$

$$j = 1, 2, \dots, n_m$$

where σ' is determined from

$$\rho \sigma'_i = \sum_{j=1}^{n_r} (\alpha''_{ij} - \alpha'_{ij}) k_{bj} \prod_{k=1}^n (\rho \sigma_k)^{\alpha''_{kj}} (\rho \sum_{k=1}^n \sigma_k)^{\alpha''_{n+1,j}} \lambda_j \quad (21)$$

$$i = n_a + 1, \dots, n$$

and

$$\sigma'_i = \sum_{j=n_a+1}^n \beta_{ij} \sigma'_j, \quad i = 1, 2, \dots, n_a \quad (22)$$

The differential equation system is now composed of Eqs. (9), (11), (20) and (22) when the area function is controlling and Eq. (18) replaces Eq. (11) in the transonic region when the Mach number is controlling.

Integration Routine

In this section and those which follow, the procedures employed in the simultaneous numerical solution of the gas dynamic and reaction kinetic equations are outlined. Flow charts indicating the detailed steps employed in the main

computer program and the various subroutines are to be found in the Appendix. A brief statement of the function of each subroutine is also included in the Appendix. All pertinent language symbols are defined in Table I "Input Format" or in Table II "Output Format".

The equation system outlined in the previous section is integrated using Hamming's modification of Milne's Predictor-Corrector procedure (Ref. 5). This procedure is a multistep method which adjusts the integration step length to conform to the desired level of accuracy in the numerical solution. The procedure was chosen because of its excellent stability and relative stability characteristics. The algorithm is as follows for the matrix differential equation

Predictor

$$P_{n+1} = y_{n-3} + \frac{4\Delta x}{3}(2y'_n - y'_{n-1} + 2y'_{n-2}) \quad (23)$$

Modifier

$$\begin{aligned} m_{n+1} &= P_{n+1} - \frac{112}{121}(P_n - C_n) \\ m'_{n+1} &= f(x_{n+1}, m_{n+1}) \end{aligned} \quad (24)$$

Corrector

$$C_{n+1} = \frac{1}{8} [9y_n - y_{n-2} + 3\Delta x(m'_{n+1} + 2y'_n - y'_{n-1})] \quad (25)$$

Final Value

$$y_{n+1} = C_{n+1} + \frac{9}{121}(P_{n+1} - C_{n+1}) \quad (26)$$

This procedure requires initially four consecutive points on the solution curve to start. The starting integration is performed by the Runge-Kutta Fourth Order Method.

The integration step size (Δx) is controlled by two input tolerances (Tol 1, Tol 2) in the following manner:

$$|(C_{n+1} + 1)(TOL 2)| < |P_{n+1} - C_{n+1}| < |(C_{n+1} + 1)(TOL 1)|, \Delta x \text{ remains as given}$$

$$|P_{n+1} - C_{n+1}| < |(C_{n+1} + 1)(TOL 2)|, \Delta x \text{ is doubled}$$

$$|P_{n+1} - C_{n+1}| > |(C_{n+1} + 1)(TOL 1)|, \Delta x \text{ is halved}$$

In order to double the step size it is necessary to have function values at seven back steps; therefore the doubling procedure can only occur every third step. In order to halve the step size, it is necessary to obtain function values between two of the stored quantities. These are obtained from the following interpolation formulae:

$$\begin{aligned} y \text{ AT } \frac{x_{n-1} + x_n}{2} = & \frac{1}{256} (80y_n + 135y_{n-1} + 40y_{n-2} + y_{n-3}) \\ & + \frac{15\Delta x}{256} (-y'_n + 6y'_{n-1} + y'_{n-2}) \end{aligned} \quad (27)$$

$$\begin{aligned} y \text{ AT } \frac{x_{n-2} + x_{n-1}}{2} = & \frac{1}{256} (12y_n + 135y_{n-1} + 108y_{n-2} + y_{n-3}) \\ & + \frac{3\Delta x}{256} (-y'_n - 18y'_{n-1} + 9y'_{n-2}) \end{aligned} \quad (28)$$

The derivatives at the interpolated positions are obtained from the differential equation system.

If after the step size is halved the resulting error still exceeds the tolerance, the step size is halved again and the Runge-Kutta integration is used for four steps. This is done because with large rates of change of derivatives normal to solution curves, the interpolation scheme becomes unstable with multiple halvings. When multiple halvings are necessary, this is noted by a statement in the output format "Runge-Kutta restart at X = ΔX =".

Round-Off Error Control

During the integration it is necessary to add small quantities to large ones and preserve accuracy. Such is the case, for instance, when the step size is very small and even though the functions and function derivatives are large, the change in a function for this particular step may also be small. If this function change were accumulated in the normal manner, it is possible that the change in the function would be lost. To prevent this from happening, double precision arithmetic is used to add changes in the function values to the functions.

Also to prevent the loss of significant figures, it is not possible to retain the quantities λ_j (Eq. (19)) as such throughout the program. Let

$\lambda = FKC - 1$. If FKC were small compared to 1 (such would be the case when the reactions are near equilibrium) calculating λ over a succession of steps might introduce a significant error. Since λ is such an integral part of the equation system this is not tolerable. Therefore, both λ and FKC are carried in the differential equation system as variables. When λ is being used "system 1" is noted in the output and when FKC is being calculated "system 2" is noted (see Fig. 1). "System 2" is in effect when $-0.1 < FKC < 0.1$.

Integration in the Transonic Region - Throat Control

Integrating the system of equations through a convergent-divergent nozzle involves not only a singularity at the sonic point (e.g., see Eq. (11), $M = 1$) but also involves handling overflow and underflow conditions since the exact choking mass flow cannot be determined "a priori". These problems are solved directly in the program without iteration or restart.

During the integration through the subsonic section of the nozzle both the Mach number and the rate of change of the Mach number with distance are checked at each step. If the Mach number exceeds $1 - EPS1$, ($EPS1$ is an input quantity which is arbitrarily small and positive) or if the slope of Mach number with distance becomes negative, the control of the differential equation system is switched from area (Eq. (11)) to Mach number (Eq. (18)), and a linear Mach number distribution with distance is prescribed. The Mach number slope used for the control is either the value at the switch point in the case where the Mach number

exceeds 1-EPSI, or the maximum Mach number slope achieved prior to switching in the case where the slope becomes negative. The Mach number control is maintained until the Mach number exceeds $1 + \text{EPS2}$ (EPS2 defined similarly to EPSI). At this point both the new area (\tilde{A}) and the new area slope (\tilde{A}') are compared to the original input quantities (A, A'). If \tilde{A} and \tilde{A}' are both within the pre-selected tolerances (DEL, DELP), the control of the differential equation system is returned to the area and the input area distribution is modified by the relation,

$$\tilde{A} = \tilde{A}_b \left(\frac{A}{A_b} \right)^{\Delta'/\Delta} \quad (29)$$

where

$$\Delta' = \tilde{A}'_b / A'_b, \quad \Delta = \tilde{A}_b / A_b$$

and b refers to conditions at the point where $M = 1 + \text{EPS2}$. This new area distribution is used from $X = X_b$ until completion of the nozzle. If \tilde{A} and \tilde{A}' are not within the preselected tolerances the Mach number control is retained and the integration is terminated at a subsequent preselected Mach number (FINALM).

Throat Study

The deck can be used to study the effect of various throat contours. As the equations are integrated through the nozzle, information is stored at a specified Mach number in the convergent section (FMI). After the initial nozzle is calculated, the program returns to the stored position and determines a hyperbolic Mach number distribution with distance (see Eq. (30) below) using the Mach number and the slope of the Mach number at this position and a prescribed supersonic Mach number (FMTS) at different downstream locations (XITS). The equation system is then integrated using the Mach number distributions to control.

$$\begin{aligned} XITS &= (KTS - JTS)DXTS + XITS \\ M &= \frac{FMI - (FMTS - FMI)(X - XI)}{(FMTS - FMI)(X - XITS)} - (X - XI) \\ &\quad \frac{(FMI'(XITS - XJ))}{X} \end{aligned} \quad (30)$$

DISCUSSION OF THE MACHINE PROGRAM

Input Description

Input Listing

The following is a listing of the necessary input for the machine program. The input format is given in Table 1. The statement numbers in the text below refer to the card numbers (first column) of Table 1.

1. The first card is the title card. The title may be any alpha numeric information desired.
2. The second card contains the numbers NA, NM and NR. NA is the number of atomic species. The phrase atomic species can be liberally interpreted and need not be rigorous chemically. For instance NO₂ could be called an atom in N₂O₄. Non-reacting species (i.e., Argon) should be treated as atomic species. NM is the number of molecular species. N = (NA + NM) is the total number of species whose maximum value is 15. NR is the number of reactions. The maximum number of reactions that can be handled is fifteen. A separate reaction should be written for each non-reacting species in the form A = A, so that the sum of the stoichiometric coefficients is zero.
3. The third card(s) contains the stoichiometric coefficients (IALP and IALPH). The columns represent the species (i) and the rows the reactions (j). The first NM reactions must be independent. The general third body is represented by a 1 in the N + 1 column on the right hand side of the matrix.
4. Beta values are listed on the fourth card(s). β_{ij} represents the number of i th atoms (rows) in the j th molecule (columns). If an inert gas is being used as an atom all the β_{ij} 's for this row would be zero.
5. The fifth card(s) contains the kinetic rate constants D, E and F. The forward rate equation is

$$K_f = DT^E \cdot e^{-F/T}$$

where D, E and F are obtained by standard fitting procedures. In the case of a non-reacting species E and F are set equal to zero while D is set equal to one.

6. The sixth card(s) contains the values of D_c , E_c and F_c used to define the equilibrium constant in the equation:

$$K_c = D_c T^{E_c} \exp(F_c/T)$$

When starting from an equilibrium position, it is important that both the starting composition and thermodynamics properties be consistent with those determined from the equilibrium constants (K_c) used in the deck. If a supplementary program is used to establish the equilibrium conditions, both this program and the kinetic program should use the same equilibrium constants. The most consistent results have been achieved by taking the equilibrium constants from the JANAF tables or NASA SP 3001 and using a least squares fit to calculate the values of D_c , E_c and F_c (Eq. (6)). When a reaction equation for a non-reacting species is present E_c and F_c are set equal to zero while D_c is set equal to one.

7. The seventh card contains a number of physical of thermodynamic constants. T_B is the reference temperature for calculating enthalpy. R is the universal gas constant, J Joule's constant and g the gravitational constant. It can be seen from the equation system that any consistent set of units may be used for a particular calculation. All that is necessary is to introduce R , J and g in the units desired. For example, if the calculation is desired in the English system, $R = 1545 \frac{\text{ft-lbf}}{\text{mole-}^{\circ}\text{R}}$, $J = 778 \frac{\text{ft-lbf}}{\text{Btu}}$ and $g = 32.174 \frac{\text{lbf}}{\text{lbm-ft}}$. If the c.g.s. system is desired $R = 8.48 \times 10^6 \frac{\text{cm-gmf}}{\text{gm-m-}^{\circ}\text{K}}$, $J = 4.27 \times 10^4 \frac{\text{gm-cm}}{\text{cal}}$ and $g = 980.67 \frac{\text{gm-cm}}{\text{gm-f-sec}^2}$.

8. The eighth card contains starting conditions and position indicators. V , T , P and $ASTART$ are the initial velocity, temperature, pressure and area, respectively. In a nozzle calculation a false position routine is used to locate the axial position of the starting area. Two X values bracketing the desired X are needed. If the initial area is in the convergent section ($FFALSE = -1.0$), the upstream bracket is the first value in the input area versus length table. If the initial area is in the divergent section ($FFALSE = +1.0$), the downstream bracket is the last value in the area table. In both cases $XMINI$ is the other bracket and must be between the point desired and the X at the minimum area.

9. The ninth card(s) contains the molecular weights, W(I). The first NA of these must be those of the atomic species. The order of the molecular weights establishes the order for the stoichiometric matrix, the specific heat tables, the heats of formation and the concentrations.
10. The tenth card lists ISIG1, a concentration indicator. If ISIG1 = 0, the following n/6 cards (n equals the total number of species) contain mass fractions. If ISIG1 = 1, the following cards contain sigmas.
11. The UPS(I)'s on card(s) 11 are the initial mass fractions (if card 10 contains a zero), or initial sigmas (if card 10 contains a one). 0.0 cannot be used for either a mass fraction or a sigma. If a negligible amount of a species is present, use sigma = 1.0×10^{-15} .
12. Card 12 contains a number of numerical control variables. XMAX is the maximum length of the nozzle desired. If $X > XMAX$, the calculation is terminated. DELX is the initial step size in the integration. The initial step size should be kept small to insure a stable start in the Runge-Kutta integration. In a normal nozzle start where the composition is either in equilibrium or close to it, a $DELX = 10^{-7}$ ft is recommended. In a combustion chamber where the composition is far removed from equilibrium and the initial derivatives may be very large, $DELX = 10^{-20}$ ft is recommended. Since the step size can double every third step, there will be no problem of excessive integration steps because of a small initial step size. TPMAX is the value of the temperature slope after the maximum temperature slope which may be used to terminate combustion chamber calculations. When $T' < TPMAX$ the calculation will terminate. $TPMAX = 0$ corresponds to equilibrium. EPS1 is the control for switching into the Mach number system. If $1 - EPS1 \leq M$ the derivative equations will be switched. EPS2 is the control for returning to the area system. When $M > EPS2 + 1$ the control will return to the area if all the criteria have been met. EPS3 is used as a control in both the supersonic combustion chamber calculation and in nozzle calculations. In the supersonic combustion chamber when the Mach number gets within EPS3 of unity (i.e., when $M < 1 + \epsilon_3$) the calculations are terminated. This is done to prevent an overflow condition when the denominator $M^2 - 1$ goes to zero. EPS3 is not used in subsonic combustion chambers. In subsonic nozzle calculations, EPS3 is used to determine when the Mach number derivative should be compared to zero. After $M > EPS3$, the Mach number slope is compared to zero to check for subcritical

mass flow rates. EPS3 is used to prevent a slight instability at the onset of a calculation from triggering an unnecessary switch to the Mach number control system. In subsonic nozzle calculations EPS3 should be set to about 5% larger than the initial Mach number. In supersonic nozzle calculations EPS3 should be set equal to -2.

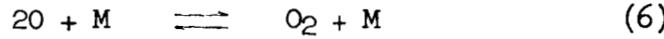
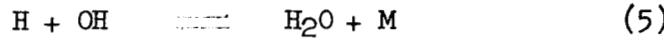
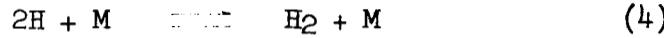
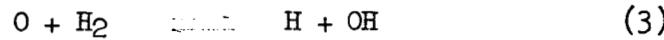
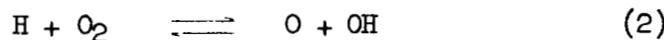
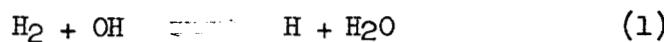
13. Additional numerical control variables are contained on card 13. DELP is the criterion for accepting slope in returning to area control and DEL is the criterion for accepting area. Both must be satisfied to return. FMMAX is the maximum Mach number desired in a given run. When $M > FMMAX$ the calculation is ended. FINALM is the maximum Mach number desired in a Mach number control system. FMI is the upstream Mach number used to initiate a throat study. XITS is the initial location downstream for the Mach number in a throat study.
14. Card 14 contains additional numerical control variables also. DXTS is the change in XITS for multiple throats. XITS is increased by DXTS for each additional throat. FLMAX is the maximum length desired for a combustion chamber. TOL 1 and TOL 2 are the upper and lower limits for step size control in the predictor-corrector integration. FLANDS is the allowable deviation from unity in the sum of the mass fractions. FMTS is the downstream Mach number for the throat study.
15. A variety of indicators appear on card 15. N1 is the number of steps skipped between prints when $M < 1 - EPS1$. N2 is the number skipped when $1 - EPS1 < M < 1 + EPS2$ and N3 is the number skipped when $M > 1 + EPS2$. NOZLNO is the number of nozzles to be calculated from a set of input. JSUPP is the print option. If JSUPP is 0, everything is printed, if it is 1, no λ , λ' predictors or correctors are printed and if it is 2, no σ , σ' , λ , λ' predictors or correctors are printed. KTS equals the number of throat studies - 1, if no throat study is to be conducted, KTS = -2. NETA establishes the mode of operation. 1 signifies a combustion chamber while 2 signifies a nozzle. NPUNO is set equal to 1 if punched cards for restart are desired, 0 if they are not. FNPNUL is the number of steps prior to the initial punch and FNPNUN2 is the number of steps skipped between punches after that.
16. Card 16 contains the geometrical constants AL and BL. The area function for a combustion chamber is; Area = AL·X + BL.

17. The heats of formation of the individual species in their standard states at the reference temperature TB are contained on card(s) 17.
18. Card(s) 18 contains the indicators, NCPl. NCPl is the number of points in each specific heat table. There must be one for each species, and $4 \leq NCPl \leq 30$.
19. The specific heat tables are contained on cards 19. The temperatures must be monatomic increasing and TB must be included in the temperature range. These tables are subsequently spline-fitted providing a third-degree polynomial between every set of points.
20. Card 20 contains IP which is the number of points in the area table ($4 \leq IP \leq 30$).
21. Card(s) 21 contain the area table. The area table is X distance versus area in which X must be monotonically increasing. This table is also fitted with a spline approximation (Ref. 6) and care should be taken in providing an even spread of points.

Sample Input

In order to illustrate the manner of use of this program as outlined in the Input Description Section, a sample calculation is described in this section for recombination of hydrogen-oxygen combustion products in a typical convergent-divergent nozzle. The combustion chamber conditions for this example are O/F = 5 and combustion pressure = 60 psia (8640 psf). The actual nozzle calculations are started downstream of the combustion chamber in the convergent section at a point where near equilibrium conditions exist and shortly upstream of the region where divergence from equilibrium is anticipated. (See section on Common Operational Problems for method of selecting the starting location.)

The reaction mechanism (i.e., the set of Eq. (12)) is:



There are two atomic species, four molecular species and six reactions. The matrix which relates the stoichiometric coefficients of the reactions (a_{ij} and c_{ij}') and the number of atoms in each of the molecules, (δ_{ij}), is given in Table II. Additional data such as initial velocity, pressure, temperature, and the thermochemical and kinetic constants are shown in Tables III-V. The English system of units is used for this calculation and the base temperature for enthalpy is 1800 °R. The area distribution must be tabulated according to step 21 of Input Description Section.

The instruction statements for a typical calculation are illustrated in the sample input sheets (Figures 1 and 2). The run is started in the convergent section of the nozzle (FALSE = -1.0) and the concentrations are in mass fractions (Table V). The switch to Mach number control is desired at a Mach number of 0.9 (EPS1 = 0.1) and the return to area control, if possible, is desired at a Mach number of 1.01 (EPS2 = 0.01). Both the area and the area slope resulting from the Mach number control integration are required to be within 10 percent (DEL = DELP = 0.1) of the input values. If they are not, the calculation will stop at a Mach number of 1.1 (FINALM = 1.1). Since no throat studies are desired, a supersonic Mach number is used for FML. An error of 5 percent (FLANDS = 0.05) will be tolerated in the sum of the mass fractions. Five steps will be skipped in the print routine in the subsonic and supersonic regimes and three will be skipped in the transonic section (N1 = 5, N2 = 3, and N3 = 5). No λ , λ' , P or C (JSUPP = 1) will be printed and cards will be punched (NPUNO = 1) every 21 steps (FNPUN2 = 20) after the first 400 (FNPUN1 = 400).

Output Description

As was indicated in the previous section, three alternative outputs are available. Selection of these outputs is controlled by the input number JSUPP. The most complete set of output data (JSUPP = 0) consists of the variables quantities listed in Table VI. Included in this print-out are the mixture velocity, temperature, pressure, density, Mach number and species concentrations as functions of axial distance. Also included are several process and geometrical variables such as the process gamma, temperature slope and the flow cross-sectional area. All of the input information discussed in the previous section is printed at the start of the calculation.

A typical sample of the complete output is included in Fig. 3.

The two abbreviated outputs retain all of the thermodynamic variables in the printout but eliminate portions of the process variables employed in the integration. Specifically, if the input number, JSUPP = 1, no λ , λ' , predictors or correctors are printed. If JSUPP = 2, no τ , σ' , λ , λ' , predictors or correctors are printed.

Common Operational Problems

The computer program as discussed previously has been used successfully for many propellant combinations over an extended period of time. During this period a great deal of experience has been gathered and some "trouble-shooting" techniques developed. Some of these techniques are presented here in order to enable more efficient use of the computer program.

Selection of Starting Location

The first problem confronting the user of this program is the selection of where to start the calculation in order to get the best results in the least amount of time. Since the deck is not designed to integrate along an equilibrium path, and since there are many more efficient ways available to perform this type of calculation, it is desirable to start the calculation from a point in the nozzle where the flow is starting to depart significantly from equilibrium flow. By making a series of very short runs at various locations in the subsonic portion of the nozzle, it is possible to locate a proper starting area. Three variables may be used to determine this starting area: the step size, DELTAX, the kinetic rate parameter, LAMBDA, or the process gamma, GAMMA-P. At equilibrium LAMBDA is equal to zero and GAMMA-P is equal to the equilibrium gamma. If a calculation is progressing along an equilibrium path, the step size will reach a constant value which is peculiar to the nozzle and which is usually quite small.

Choice of Critical Mass Flow Rate

A second problem usually encountered is the choice of the critical mass flow rate for a given nozzle with a given propellant combination. The mass flow rate of the reacting gas mixture under consideration must be between that for equilibrium flow and that for frozen flow. The critical mass flow which can vary as much as five percent for the extreme gas models is dependent on the chamber pressure and the initial Mach number of the kinetic flow calculations. As the chamber pressure increases, the mass flow must approach the equilibrium value. The hydrogen-oxygen propellant for which extensive kinetic flow calculations have been performed may be used as an example. If the chamber pressure is 300 psia, the expansion process should be essentially an equilibrium process (high chamber pressure minimizes nonequilibrium losses), and thus the flow rate should be that for equilibrium flow through the nozzle throat. When the pressure is 60 psia, the mass flow rate approaches a value 0.5 percent less than the frozen value, i.e., near frozen mass flow.

Also the nearness to a Mach number of unity for the starting Mach number affects the choking mass flow rate. Since the flow is in equilibrium at the start,

as the area of the start gets closer to the sonic point the mass flow rate must lie nearer to the equilibrium value.

In general, it will be difficult to guess the mass flow rate that corresponds to a particular nozzle, especially if the expansion characteristics of the combustion products of the propellant combination are unfamiliar. For initial attempts to match throat contours, the nozzle produced in system 2 (see throat calculation) will probably not meet the area and the area slope tolerances. Corrections can be made without rerunning the entire subsonic nozzle at a new mass flow rate. If the produced nozzle has a slope greater than desired, it may be corrected by rerunning the case from a Mach number lower than the original switch point with the new EPS1 equal to a larger value than the original. This will cause the transfer to the Mach number control system to occur when the Mach number derivative is smaller and the nozzle produced will have less curvature than the first attempt. It is also possible in many cases that the produced nozzle can be combined graphically with the desired nozzle in such a way that a new nozzle very similar to the original desired nozzle is produced. The latter can then be input and the case restarted in the supersonic portion.

Aborted Starting

Sometimes without apparent reason a calculation may terminate almost as soon as it starts. This termination may be caused, on the surface, by the sum of the mass fractions exceeding the limit, by the temperature being outside the table range or by an error routine, such as negative square root, being triggered. If, after a careful check of the input, nothing appears to be incorrect, a strong possibility may be that the initial step size was too large. Too large an initial step size causes an unstable Runge-Kutta integration which can, in turn, result in all of the errors mentioned above. If this happens, the calculation should be rerun with the initial step size set to 10^{-20} feet, this will allow the calculation to get past the Runge-Kutta integration and in general continue without further trouble. The step size will rapidly build up to an acceptable value.

Machine Overflow

Another minor source of trouble has been a machine overflow condition in the supersonic portion of the flow. This is generally caused by the exponential term in the rate constant equation ($\exp(F/T)$). F is often a large number (1.0×10^6) and when T becomes small, such as in a large area ratio nozzle, the resulting F/T may overflow the machine. When this happens, the flow is invariably frozen. If continued running is desired, the value of F may be modified without affecting the results so that it no longer causes an overflow. However, if the flow is still reacting, it will be necessary to refit the rate equation for a lower temperature range to overcome this problem.

REFERENCES

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3. Investigation of Nonequilibrium Flow Effects in High Expansion Ratio Nozzles. Quarterly Progress Report No. 2 under Contract NAS3-2572. United Aircraft Corporation Research Laboratories Report C910096-6, March 18, 1964.
4. Investigation of Nonequilibrium Flow Effects in High Expansion Ratio Nozzles. Quarterly Progress Report No. 3 under Contract NAS3-2572. United Aircraft Corporation Research Laboratories Report C910096-9, June 18, 1964.
5. Hamming, R. W.: Stable Predictor Corrector Methods for Ordinary Differential Equations. Journal Association Computing Machinery, Vol. 6, 1959.
6. Ahlberg, J. H., and E. Nilson: Convergence Properties of the Spline Fit. Journal of the Society of Industrial and Applied Mathematics, Vol. 11, No. 1, March 1963.

LIST OF SYMBOLS

| | |
|-------------|---|
| A | Area |
| \tilde{A} | Area (transonic region) |
| C | Velocity of sound |
| c_{pi} | Specific heat |
| D | Forward rate constant coefficient |
| D_c | Equilibrium constant coefficient |
| E | Forward rate coefficient |
| E_c | Equilibrium constant coefficient |
| F | Forward rate coefficient |
| F_c | Equilibrium constant coefficient |
| g | Gravitational constant |
| H | Enthalpy |
| H_{fi} | Heat of formation of ith component |
| h_i | Enthalpy of ith component |
| H_0 | Stagnation enthalpy |
| J | Mechanical equivalent of heat energy |
| K_f, K_b | Specific reaction rate constants, forward reactions and reverse reactions |
| K_c | Equilibrium constants in concentration units |
| M | Mach number |
| \dot{m}^c | Mass flow rate |

LIST OF SYMBOLS (Cont.)

| | |
|--------------------|--|
| P | Pressure |
| R | Universal gas constant |
| T | Temperature |
| V | Velocity |
| x | Length |
| a_{ij}, a''_{ij} | The stoichiometric coefficients, of the i th species in the j th reaction, reactants and products, respectively. |
| β_{ij} | The number of the i th atomic species in the j th molecular species |
| γ | Ratio of specific heats defined by equation 5a |
| λ | Variable defined by equation 18 |
| ρ | Density |
| σ | Concentration: mass fraction divided by molecular weight |

Subscripts

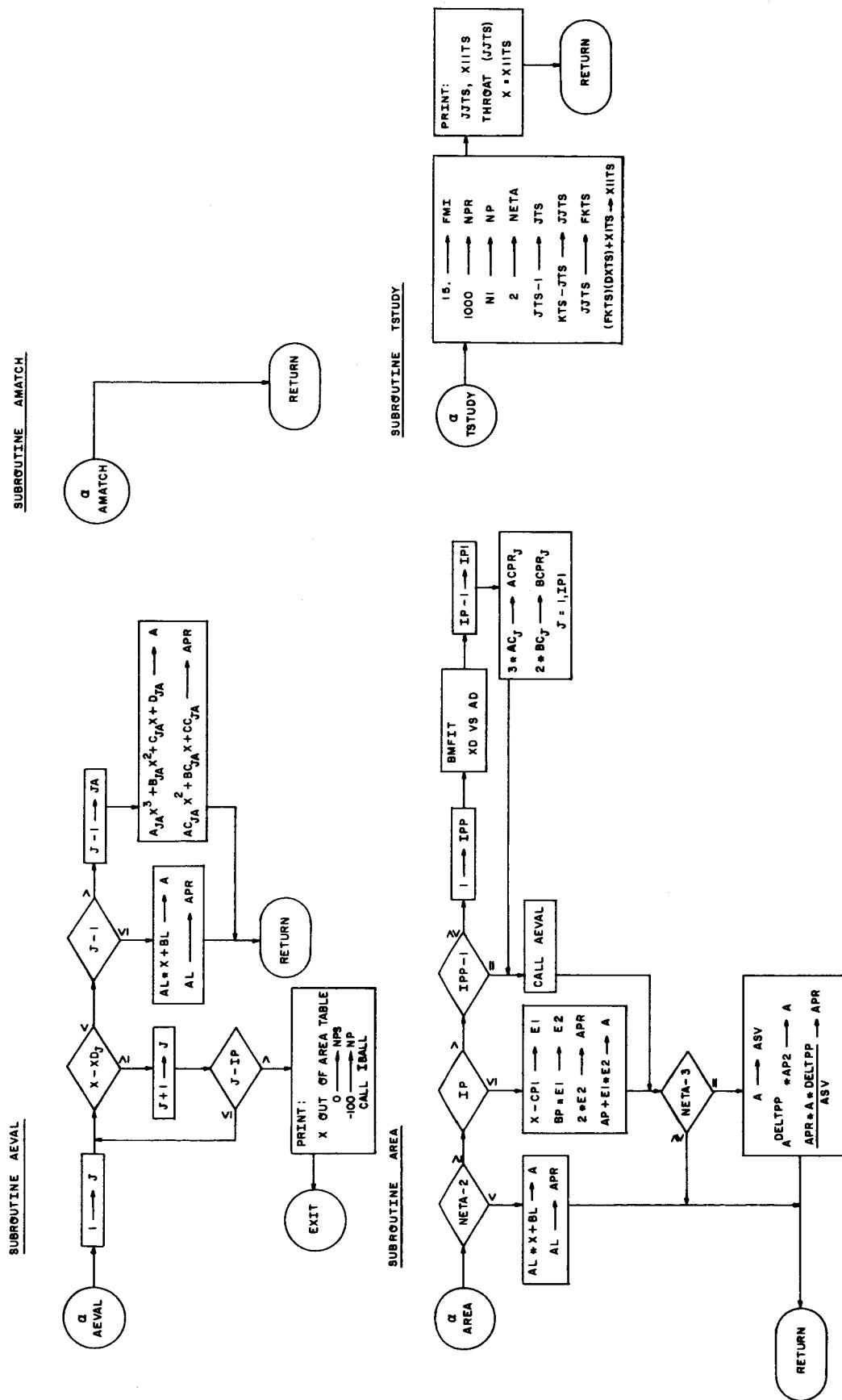
| | |
|-----------|---|
| b | Indicates reference base or backward chemical change |
| f | Indicates forward reaction rate |
| i, j, k | Indices used interchangeably to signify atoms, species or reactions in generalized analytical expressions |
| n_a | Number of atomic species |
| n_m | Number of independent chemical reactions |
| n_r | Total number of chemical reactions |
| o | Stagnation conditions |

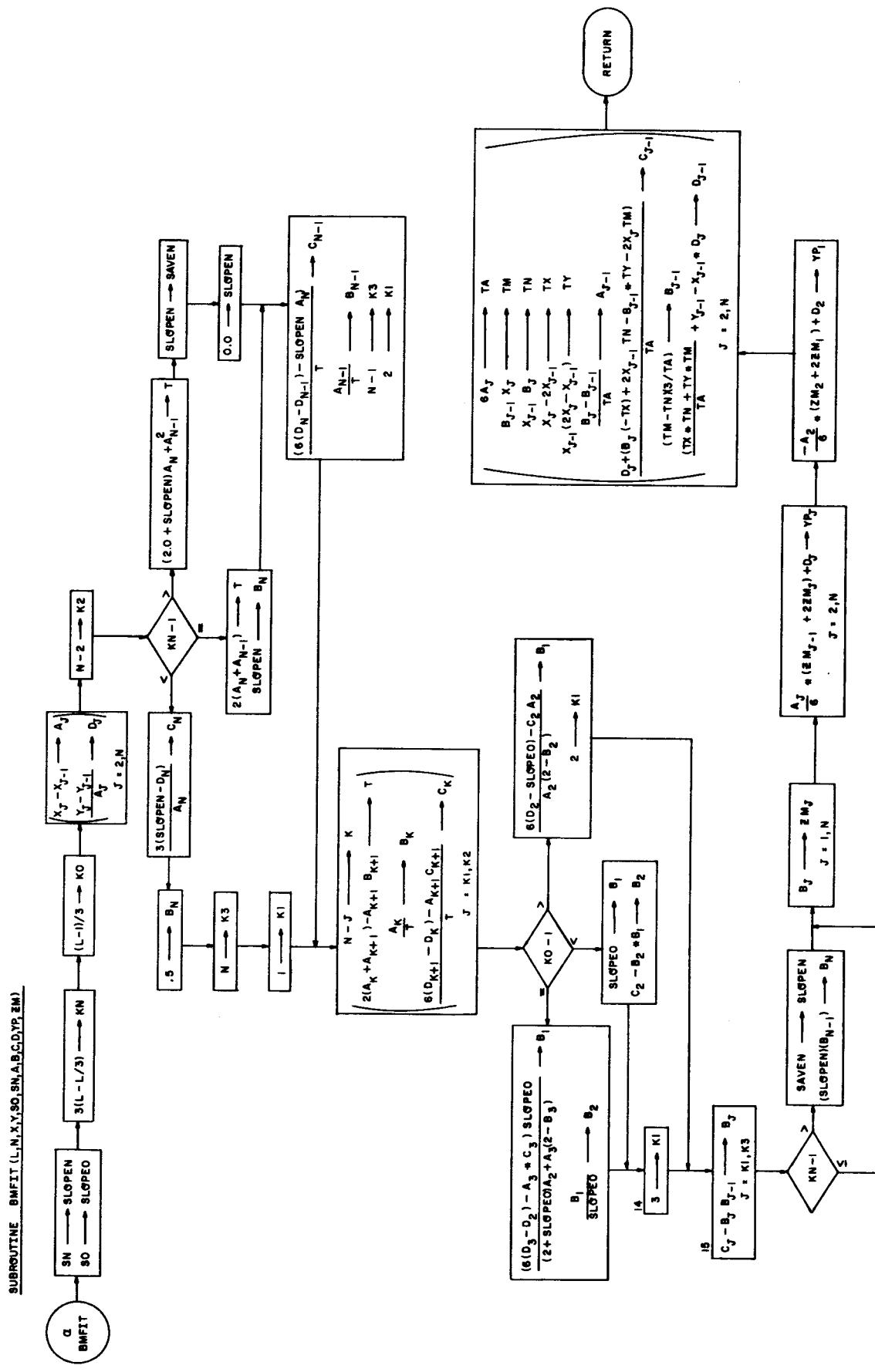
LISTING OF SUBROUTINES AND FLOW CHARTS

The following is a listing of subroutines which comprise the IBM 7094 computer program for solving the one-dimensional gas dynamic and chemical kinetic equations. The flow charts for these subroutines are included immediately after the listing in Figs. I-1 through I-15.

- AEVAL** (Fig. I-1) - Evaluates the area at a given X by using a cubic equation.
- AMATCH** (Fig. I-1) - Is a dummy subroutine.
- AREA** (Fig. I-1) - Obtains cubic coefficients of the A vs X table by using BMFIT.
- BMFIT** (Fig. I-2) - Fits tabular data by forming coefficients between tabular data points. For some interval such that $X_i < X < X_{i+1}$ we can obtain $f(X) = a_i X^3 + b_i X^2 + c_i X + d_i$, where a_i , b_i , c_i and d_i are the generated coefficients.
- BOSS** (Fig. I-3,4) - Is the controlling subroutine of the entire program. It determines, by using various checks, when each of the other subroutines should be used.
- CPHVAL** (Fig. I-5) - Evaluates C_p , h , and $\frac{dC_p}{dT}$ at a given T by using a cubic equation.
- CPUFIT** (Fig. I-6) - Reads cards of Number 18 and Number 19. These cards are the C_p vs T table. By using BMFIT it obtains cubic coefficients for each C_p vs T table and integrates C_p to obtain h .
- DERIV** (Fig. I-7,8) - Computes the values of T' , p' , σ' , and λ' in the differential equation system. This routine is used by both HAM and KUTTA.
- FALSIE** (Fig. I-9) - Uses the method of false position to converge on the root of an equation.
- FZERO** (Fig. I-10) - Defines the equation which enables the program to converge to the proper starting X_1 value. It is used exclusively by FALSIE.
- HAM** (Fig. I-11) - Is Hamming's method for integrating a system of differential equations. Hamming's method uses predictor-corrector steps.

- IBALL** (Fig. I-12) - Stores and prints all output while the program is in execution.
- INPUT** (Fig. I-10) - Reads and prints cards of Number 1 through Number 17.
- INVERT** (Fig. I-13) - Inverts a matrix. In this program it is used to invert the stoichiometric matrix.
- KUTTA** (Fig. I-14) - Integrates a system of differential equations using a Runge-Kutta type of integration scheme. It is used for starting the program and making various restarts.
- MAIN** (Fig. I-15) - Is the calling program for INPUT, CPUFIT, and BOSS.
- NUNOZL** (Fig. I-5) - Reads cards of Number 20 and Number 21. This is the A vs X table.
- QUITI** (Fig. I-5) - Is used to stop a combustion chamber run. It checks input quantities against generated variables and stops if the input quantities have been exceeded.
- START** (Fig. I-15) - Obtains, by using a Runge-Kutta integration scheme, the initial four points necessary to use Hamming's method of integration.
- TRNSFM** (Fig. I-15) - Determines whether our differential equation system will be in λ or $\lambda + 1$. This is done to prevent taking the natural log of 0.
- TSTUDY** (Fig. I-1) - Controls variable changes which allow multiple throat studies.





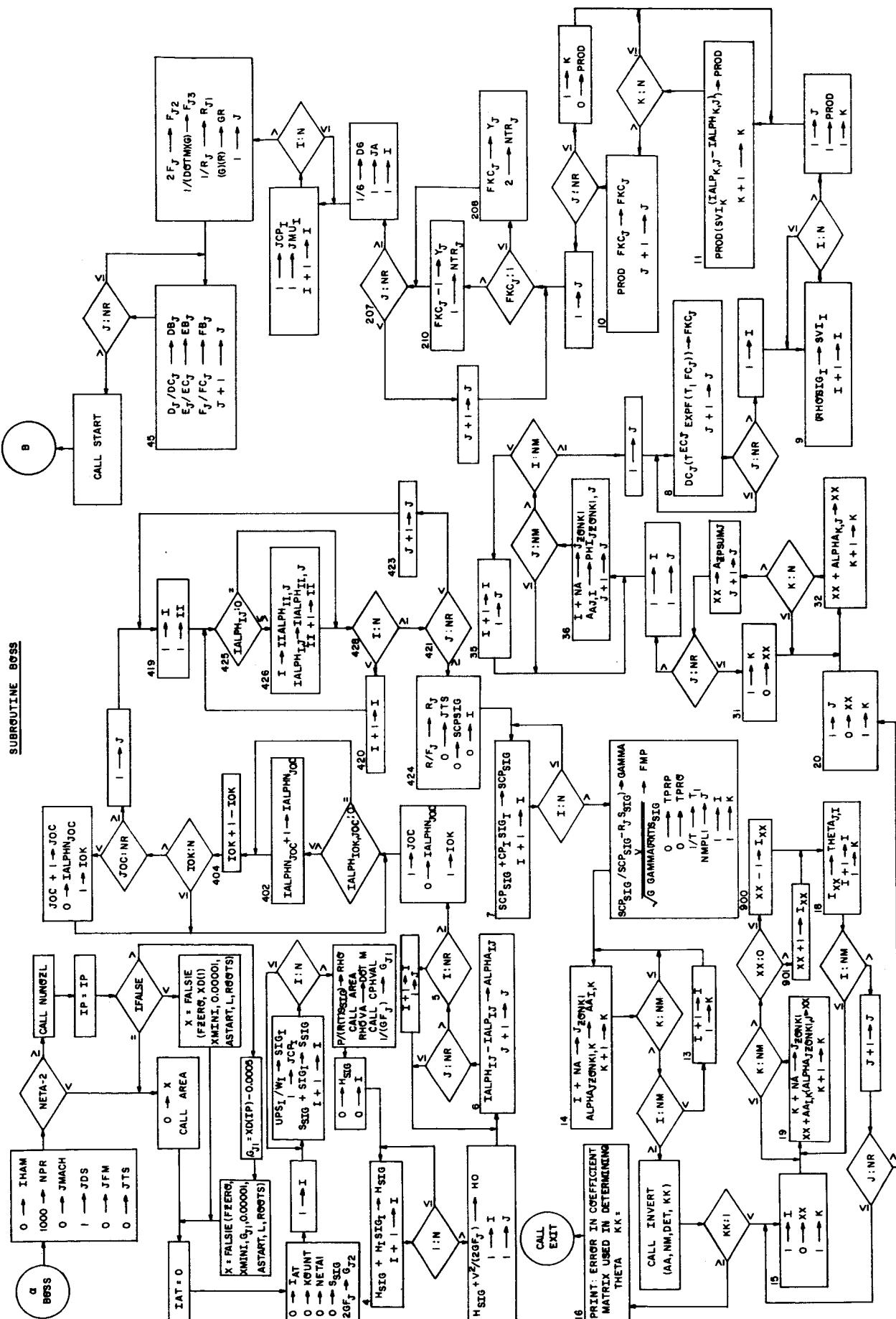
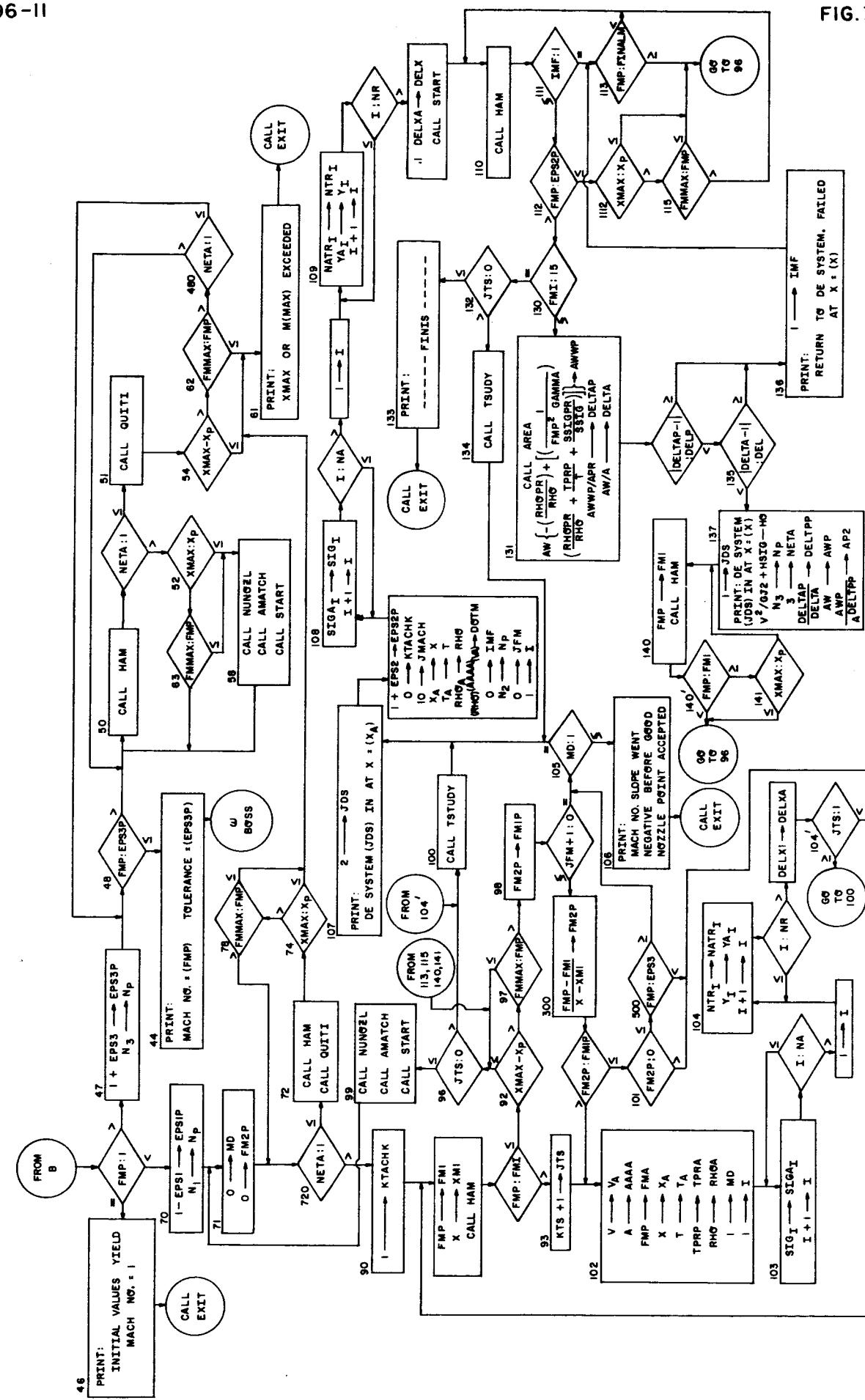


FIG. I-4



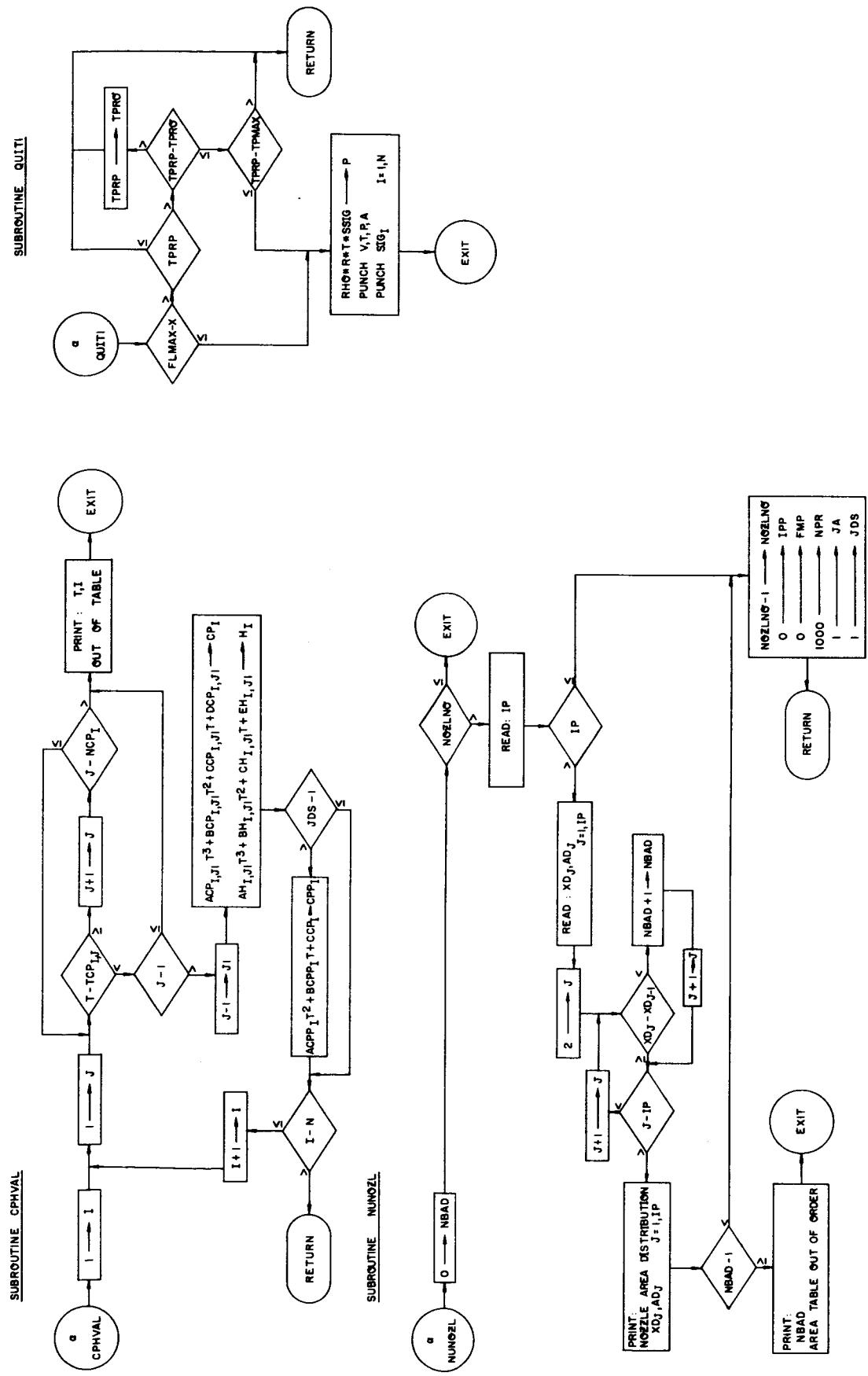
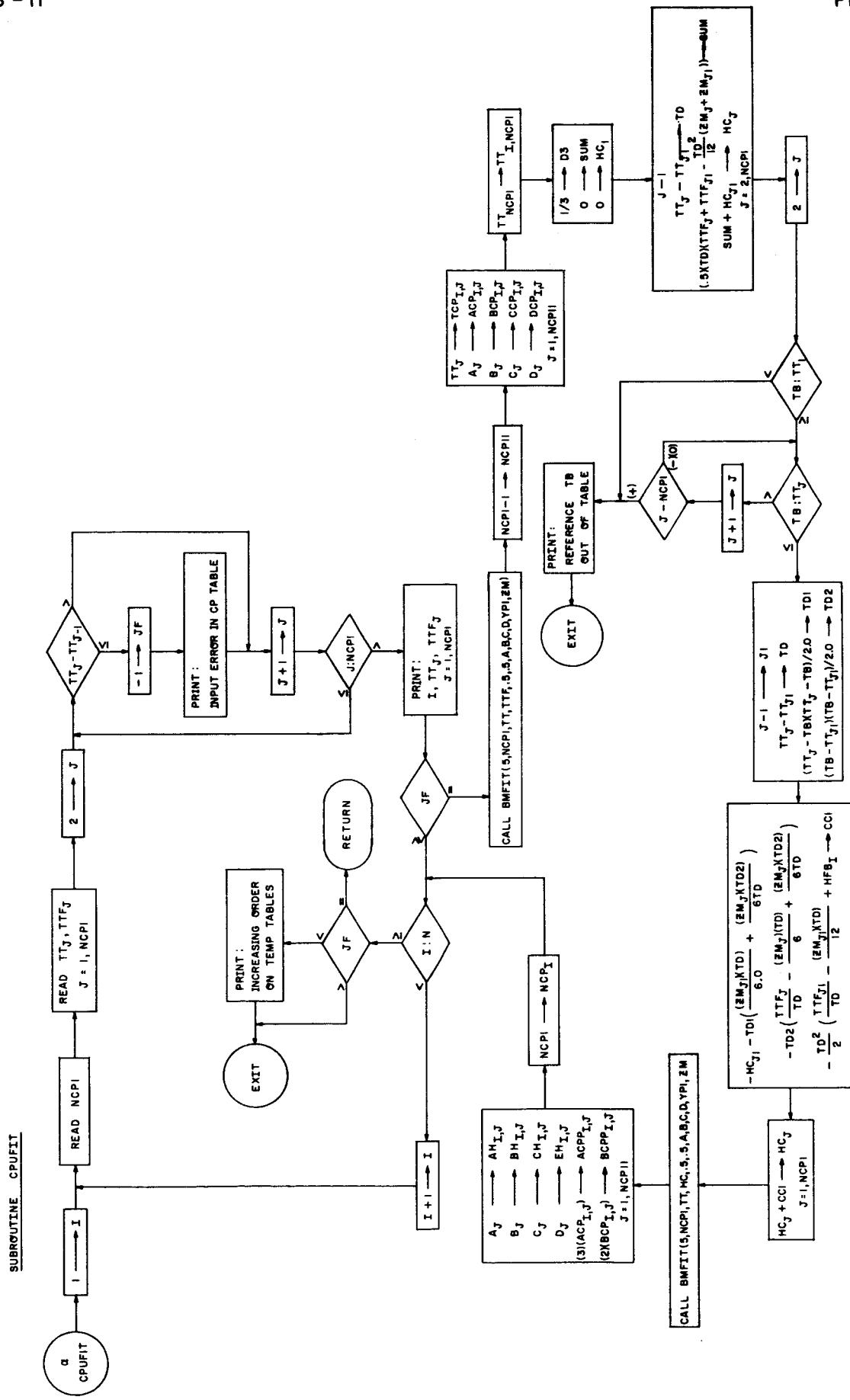
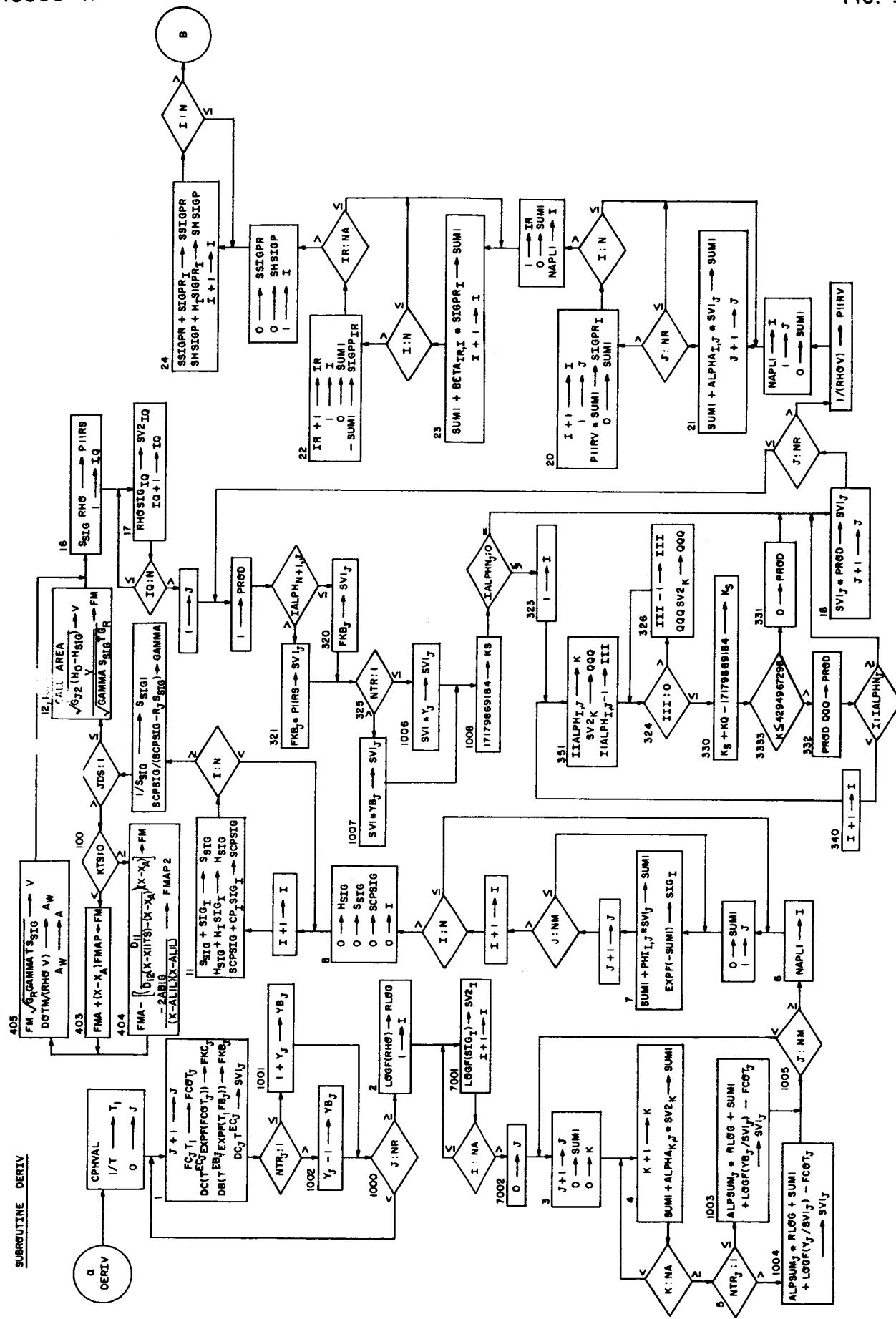
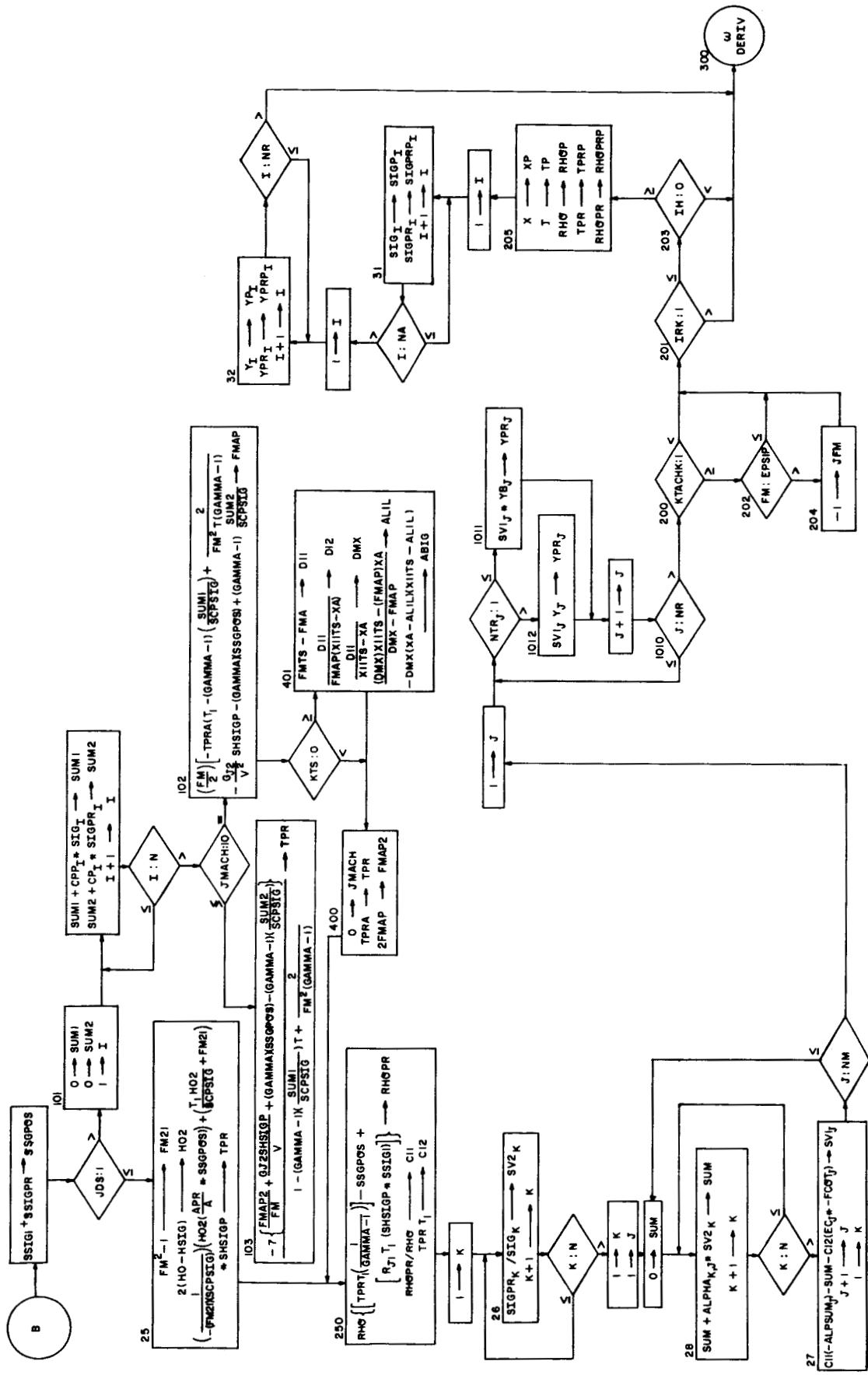


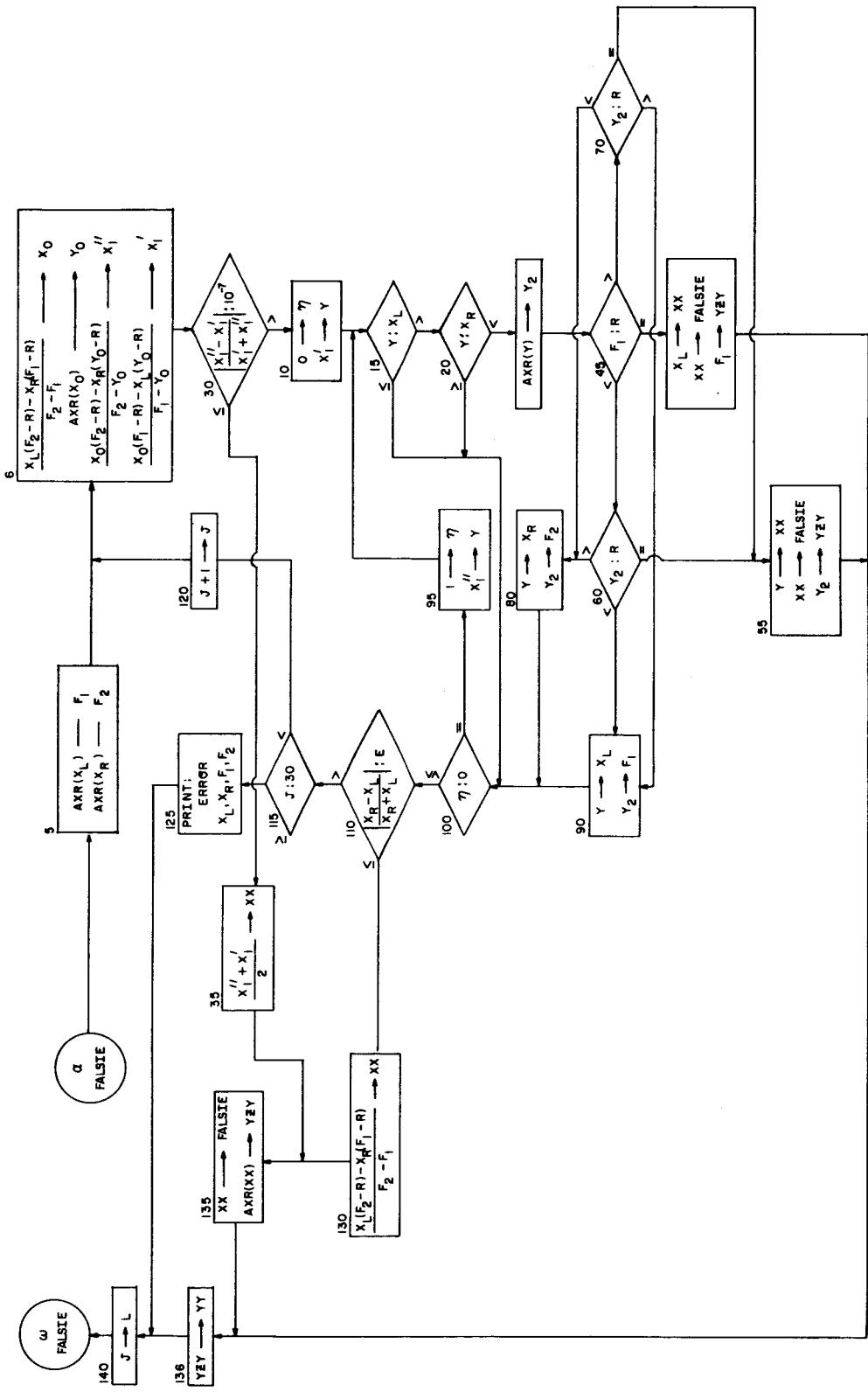
FIG. I-6





SUBROUTINE DERIV (CONT'D)



SUBROUTINE FALSIE (AXR, X_L, X_R, E, R, L, YY)

NOTE : AXR ≡ FUNCTION SUBROUTINE

FIG. I-10

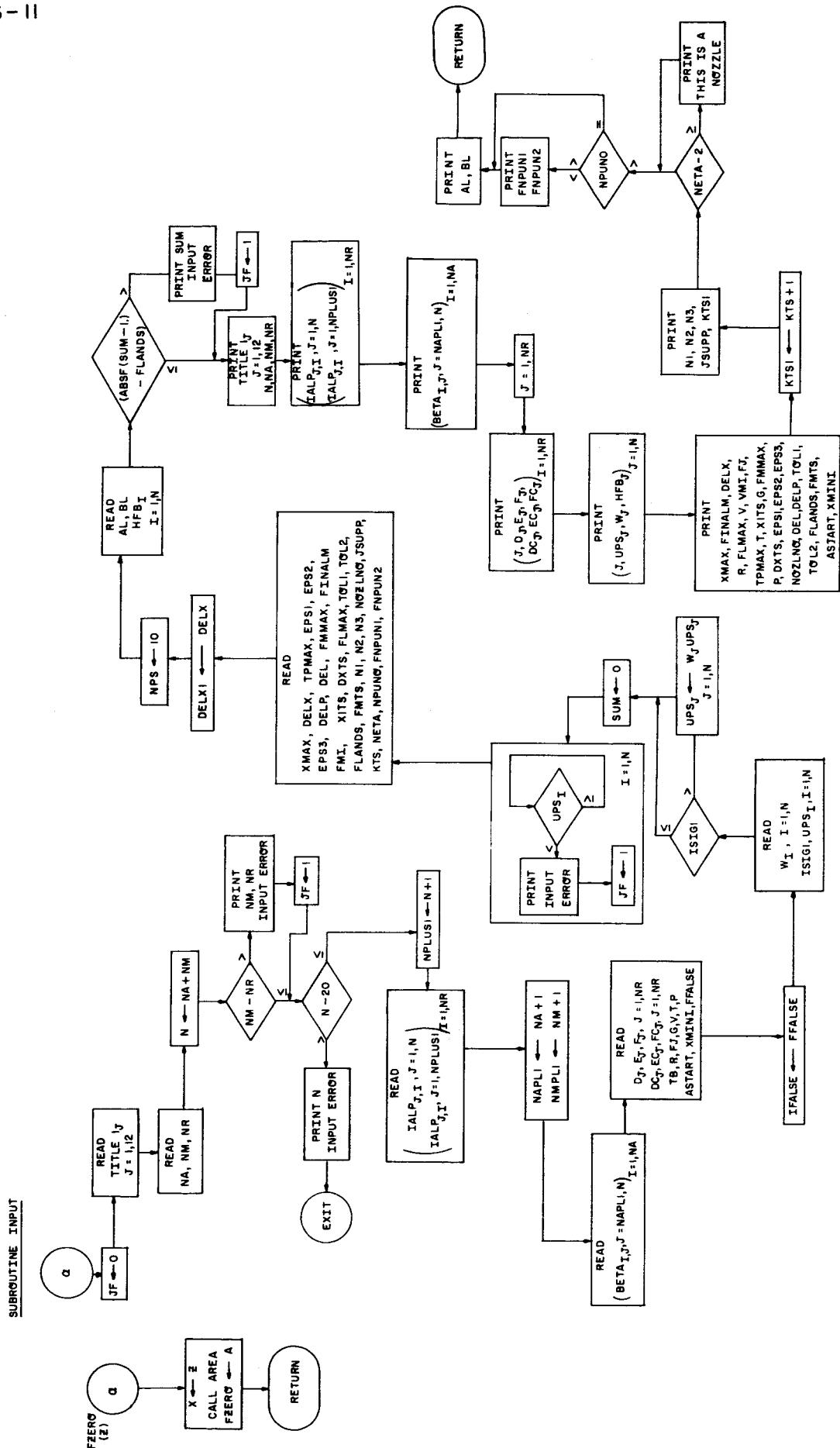
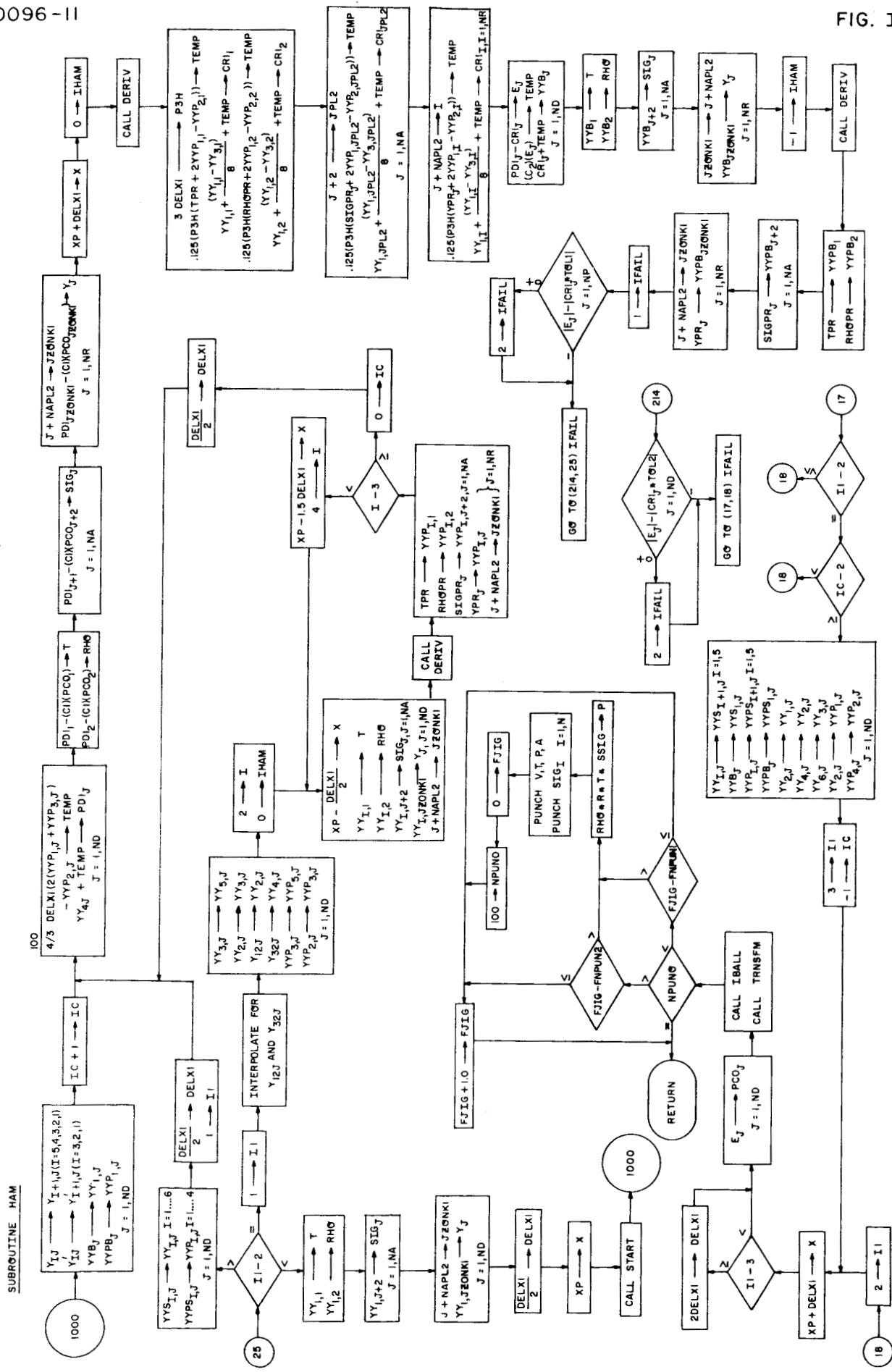
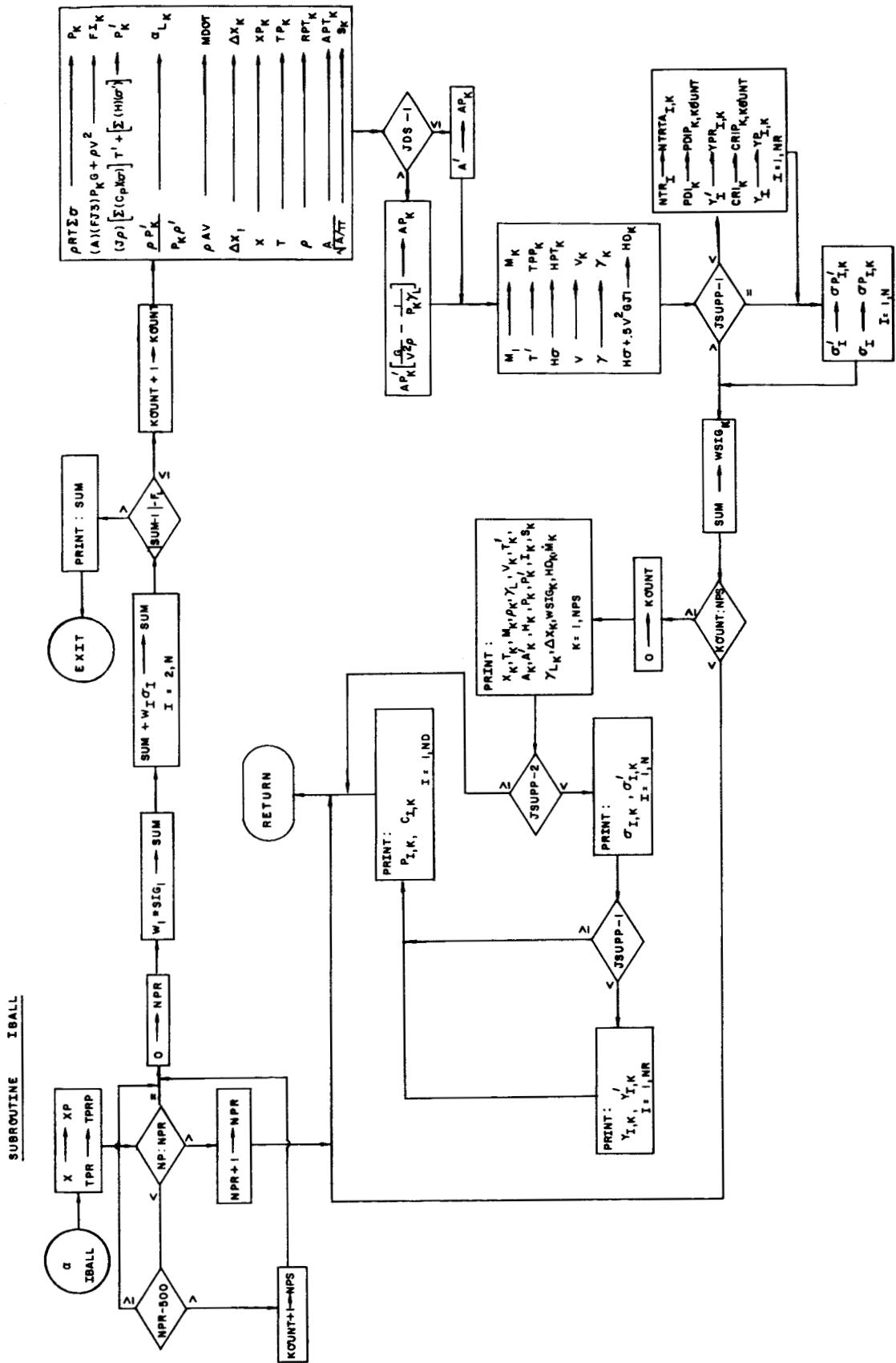
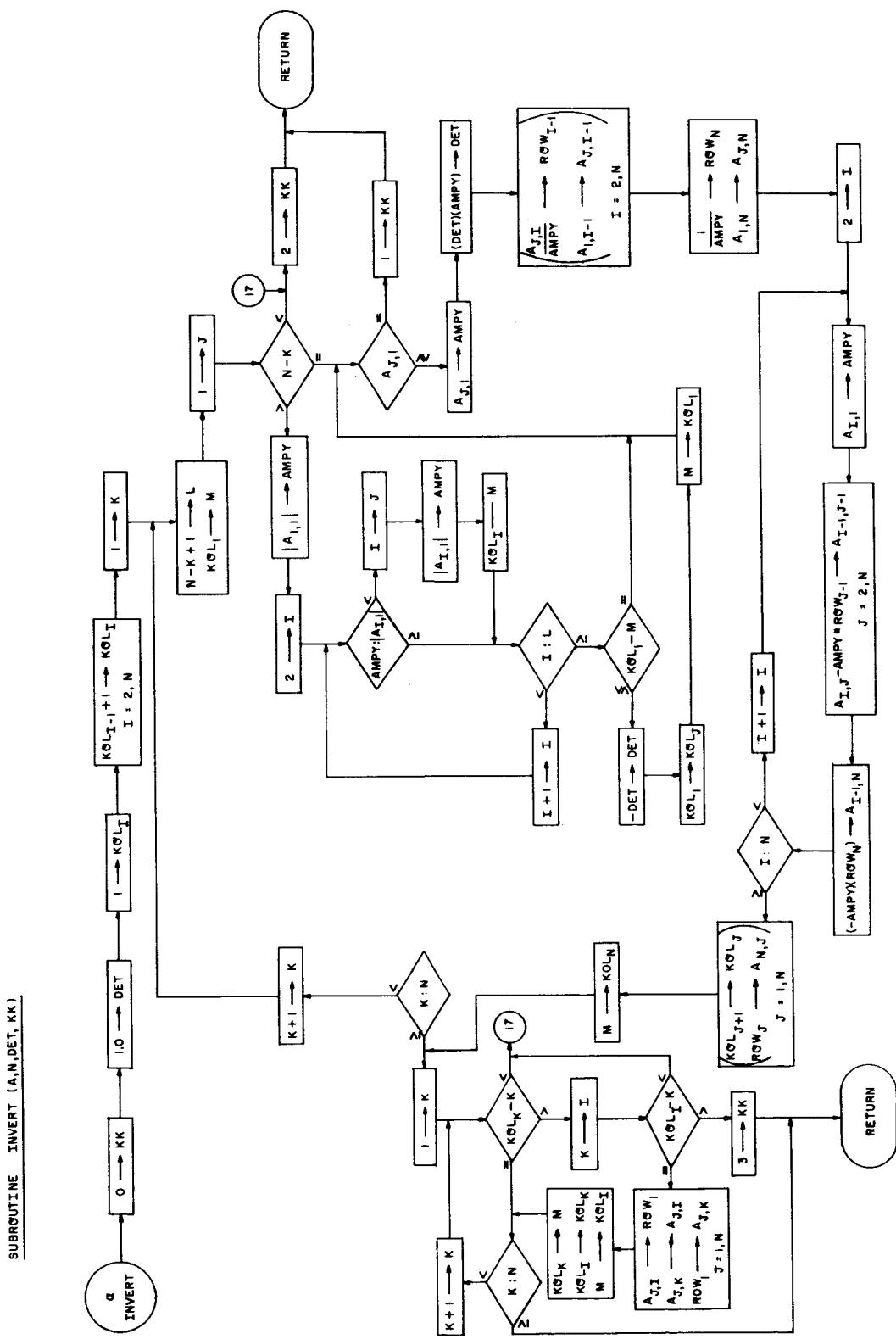


FIG. I-II







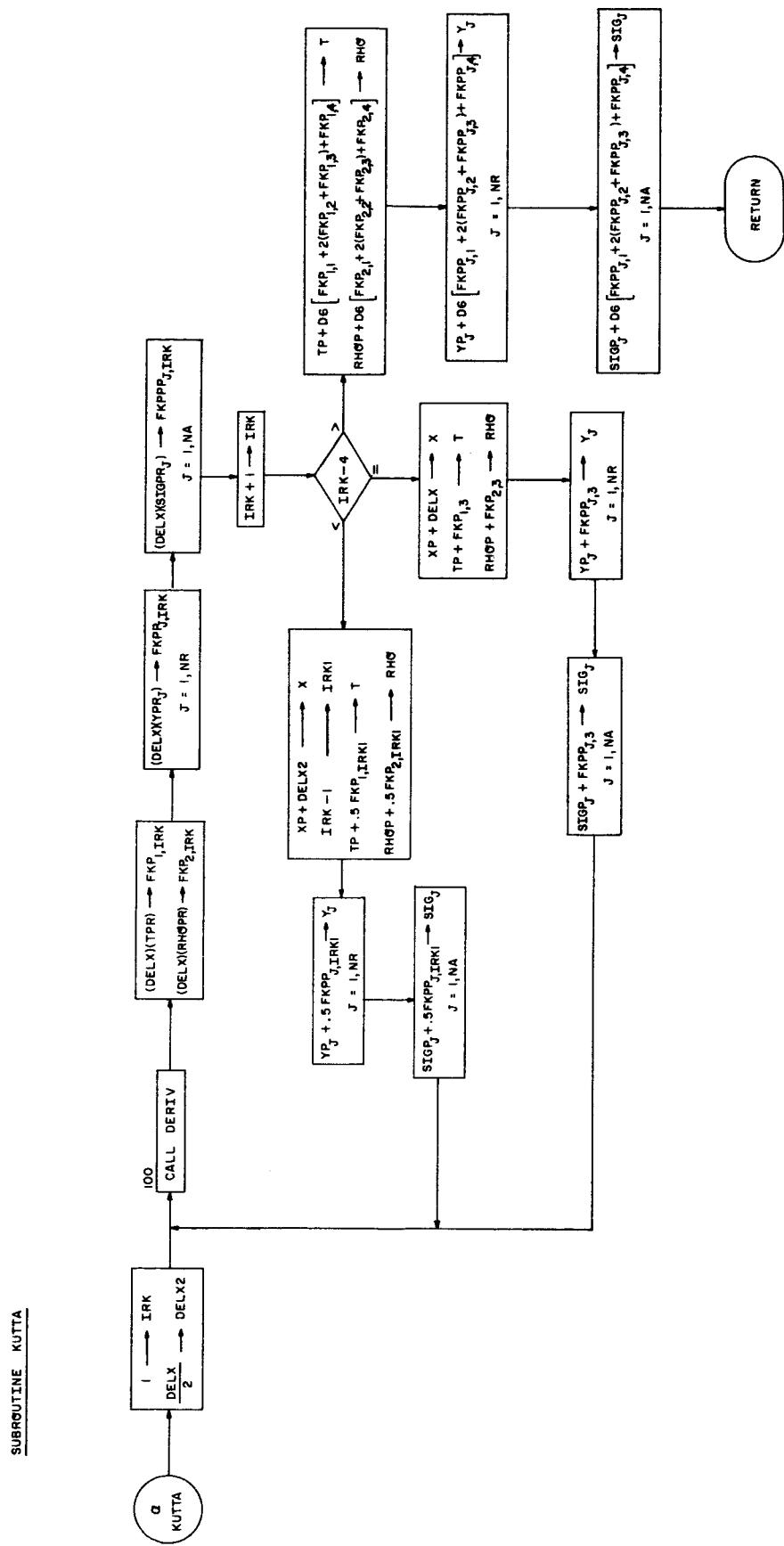
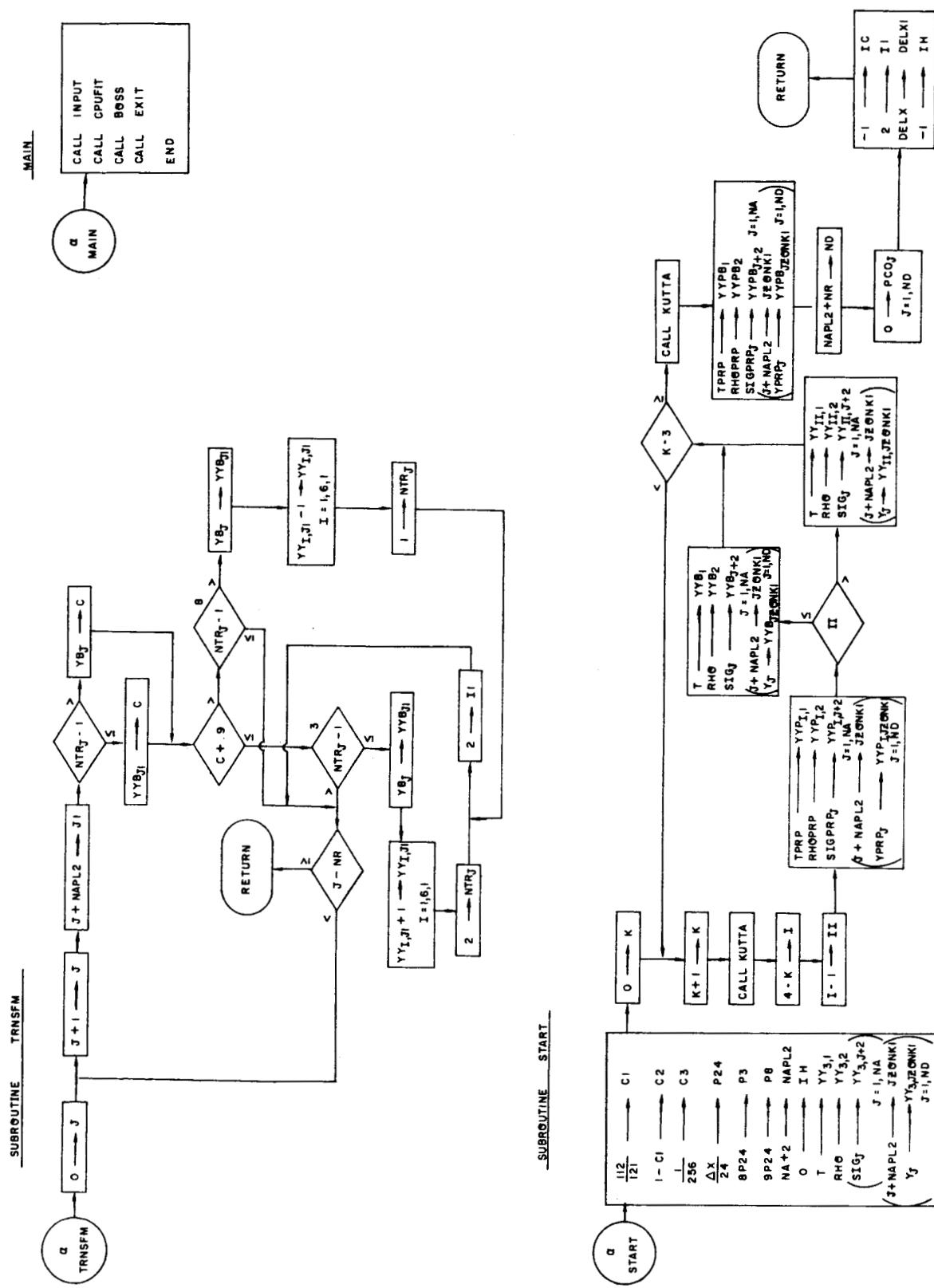


FIG. I-15



APPENDIX II

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TABLE I

Input Format

| <u>Number</u> | <u>Number of Cards</u> | <u>IBM Fortran Format</u> | <u>Columns Used</u> | <u>Description</u> | <u>Nomenclature</u> |
|---------------|------------------------|---------------------------|---------------------|--------------------|----------------------------------|
| 1 | 1 | A | 2-72 | Title | |
| 2 | 1 | 3I3 | 1-3 | NA | Atomic Species |
| | | | 4-6 | NM | Molecular Species |
| | | | 7-9 | NR | Reactions |
| 3 | NR | 1X, 4I11 | 2-16 | IALP (J,I) | Stoichiometric Coefficients |
| | | | 17-32 | IALPH (J,I) | Stoichiometric Coefficients |
| 4 | NA | 1X, 15F1.0 | 2-16 | BETA (I,J) | Number of atoms in molecule |
| 5 | NR/2 | 6E12.7 | 1-12 | D (J) | Constant in Rate Equation |
| | | | 37-48 | | |
| | | | 13-24 | E (J) | Constant in Rate Equation |
| | | | 49-60 | | |
| | | | 25-36 | F (J) | Constant in Rate Equation |
| | | | 61-72 | | |
| 6 | NR/2 | 6E12.7 | 1-12 | DC (J) | Constant in Equilibrium Equation |
| | | | 37-48 | | |
| | | | 13-24 | EC (J) | Constant in Equilibrium Equation |
| | | | 49-60 | | |
| | | | 25-36 | FC (J) | Constant in Equilibrium Equation |
| | | | 61-72 | | |

TABLE I
(Cont.)

| <u>Number</u> | <u>Number of Cards</u> | <u>IBM Fortran Format</u> | <u>Columns Used</u> | <u>Description</u> | <u>Nomenclature</u> |
|---------------|------------------------|---------------------------|---------------------|--------------------|--------------------------|
| 7 | 1 | 6E12.7 | 1-12 | TB | Base Temperature |
| | | | 13-24 | R | Gas Constant |
| | | | 25-36 | FJ | Joules Constant |
| | | | 37-48 | G | Gravity Constant |
| 8 | 1 | 6E12.7 | 1-12 | V | Velocity |
| | | | 13-24 | T | Temperature |
| | | | 25-36 | P | Pressure |
| | | | 37-48 | ASTART | Starting Area |
| | | | 49-60 | XMINI | False position bracket |
| | | | 61-72 | FFALSE | False position indicator |
| 9 | N/6 | 6E12.7 | 1-12 | W (I) | Molecular weight |
| | | | ↓ | | |
| | | | 61-72 | | |
| 10 | 1 | I3 | 3 | ISIG1 | Indicator |
| 11 | N/6 | 6E12.7 | 1-12 | UPS (J) | Concentrations |
| | | | ↓ | | |
| | | | 61-72 | | |
| 12 | 1 | 6E12.7 | 1-12 | XMAX | Maximum length |
| | | | 13-24 | DELX | Initial step size |

TABLE I
(Cont.)

| <u>Number</u> | <u>Number of Cards</u> | <u>IBM Fortran Format</u> | <u>Columns Used</u> | <u>Description</u> | <u>Nomenclature</u> |
|---------------|------------------------|---------------------------|---------------------|--------------------|---------------------------------|
| | | | 25-36 | TPMAX | Temperature slope in combustion |
| | | | 37-48 | EPS1 | Indicator |
| | | | 49-60 | EPS2 | Indicator |
| | | | 61-72 | EPS3 | Indicator |
| 13 | 1 | 6E12.7 | 1-12 | DELP | Slope tolerance |
| | | | 13-24 | DEL | Area tolerance |
| | | | 25-36 | FMAX | Maximum Mach no. |
| | | | 37-48 | FINALM | Maximum Mach No. system 2 |
| | | | 49-60 | FMI | Throat study Mach number |
| | | | 61-72 | XITS | Throat study location |
| 14 | 1 | 6E12.7 | 1-12 | DXTS | Change in XITS |
| | | | 13-24 | FLMAX | Maximum length combustion |
| | | | 25-36 | TOLL | Integration tolerance |
| | | | 37-48 | TOL2 | Integration tolerance |
| | | | 49-60 | FLANDS | Mass fraction tolerance |
| | | | 61-72 | FMTS | Throat study Mach number |
| 15 | 1 | 8I3, 2E6.0 | 1-3 | N1 | Print indicator |
| | | | 4-6 | N2 | Print indicator |
| | | | 7-9 | N3 | Print indicator |

TABLE I
(Cont.)

| <u>Number</u> | <u>Number of Cards</u> | <u>IBM Fortran Format</u> | <u>Columns Used</u> | <u>Description</u> | <u>Nomenclature</u> |
|---------------|------------------------|---------------------------|---------------------|--------------------|-----------------------------|
| | | | 10-12 | NOZLNO | Number of nozzles |
| | | | 13-15 | JSUPP | Print option |
| | | | 16-18 | KTS | Throat study indicator |
| | | | 19-21 | NETA | Mode of operation indicator |
| | | | 22-24 | NPUNO | Punch indicator |
| | | | 25-30 | FNPUN1 | Punch indicator |
| | | | 31-36 | FNPUN2 | Punch indicator |
| 16 | 1 | 6E12.7 | 1-12 | AL | Area constant |
| | | | 13-24 | BL | Area constant |
| 17 | N/6 | 6E12.7 | 1-12 | HFB (I) | Heat of formation |
| | | | ↓ | | |
| | | | 61-72 | | |
| 18 | N | I3 | 2,3 | NCPl | Indicator |
| 19 | NCPl/3 | 6E12.7 | 1-12 | | |
| | | | 25-36 | TT (J) | Temperature |
| | | | 49-60 | | |
| | | | 13-24 | TTF (J) | Specific heat |
| | | | 37-48 | | |
| | | | 61-72 | | |

TABLE I
(Cont.)

| <u>Number</u> | <u>Number of Cards</u> | <u>IBM Fortran Format</u> | <u>Columns Used</u> | <u>Description</u> | <u>Nomenclature</u> |
|---------------|------------------------|---------------------------|---------------------|--------------------|---------------------|
| 20 | 1 | I12 | 11,12 | IP | Indicator |
| 21 | IP | 2E12.3 | 1-12 | XD (J) | Axial Distance |
| | | | 13-24 | AD (J) | Area |

TABLE II

Sample Input - Species Matrices $\alpha'_{ij}, \alpha''_{ij}, \beta_{ij}$

| α'_{ij} Matrix (Reactants) | | | | | | | α''_{ij} Matrix (Products) | | | | | | |
|-----------------------------------|---|---|----------|----------|----------|----------|-----------------------------------|---|-------|-------|----|--------|---|
| Reaction (J) | O | H | O_2 | H_2 | OH | H_2O | Species (i) | | | | | | |
| | - | - | <u>-</u> | <u>-</u> | <u>-</u> | <u>-</u> | O | H | O_2 | H_2 | OH | H_2O | M |
| (1) | 0 | 0 | 0 | 1 | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 |
| (2) | 0 | 1 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 |
| (3) | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 1 | 0 | 0 | 1 | 0 | 0 |
| (4) | 0 | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 1 |
| (5) | 0 | 1 | 0 | 0 | 1 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 1 |
| (6) | 2 | 0 | 0 | 0 | 0 | 0 | 0 | 0 | 1 | 0 | 0 | 0 | 1 |

 β_{ij} Matrix (Atom Balance)

| Atoms (i) | Molecules (j) | | | |
|-----------|---------------|---------|--------|----------|
| | (O_2) | (H_2) | (OH) | (H_2O) |
| (O) | 2 | 0 | 1 | 1 |
| (H) | 0 | 2 | 1 | 2 |

TABLE III

Sample Input - Forward Reaction Rates*

$$K_f = DT^E e^{F/T}$$

| Reaction | D | E | F |
|----------|------------|-------------|-------------|
| 1 | 0.50300E11 | 0.50000E00 | -0.90500E04 |
| 2 | 0.90600E12 | 0. | -0.13700E05 |
| 3 | 0.19280E12 | 0. | -0.83400E04 |
| 4 | 0.23555E18 | -0.14998E01 | -0.14930E04 |
| 5 | 0.17268E17 | -0.10900 | 0.53750E04 |
| 6 | 0.63684E14 | -0.50000E00 | 0. |

* Units: lbs moles, ft³, °R, sec

TABLE V

Sample Input - Starting Conditions

$T_b = 1800^{\circ}\text{R}$
 $R = 1545.4 \frac{\text{ft} - \text{lbf}}{\text{lbfm}^{\circ}\text{R}}$
 $J = 778.2 \frac{\text{ft} - \text{lbf}}{\text{Btu}}$
 $g = 32.174 \frac{\text{lbfm} - \text{ft}}{\text{lbf} - \text{sec}^2}$
 $V = 3232.1 \frac{\text{ft}}{\text{sec}}$
 $T = 5383.0^{\circ}\text{R}$
 $P = 6912.0 \frac{\text{lbf}}{\text{ft}^2}$
 $A_{\text{START}} = .0107686 \text{ ft}^2$
 $X_{\text{MIN}} = .04611665 \text{ ft}$

| Species | Molecular Weights | Initial Mass Fractions | $\frac{\text{lbfm}}{\text{lbfm Total}}$ |
|----------------------|-------------------|------------------------|---|
| O | 16.0 | 0.0032815333 | |
| H | 1.008 | 0.0043441212 | |
| O_2 | 32.0 | 0.0043577911 | |
| H_2 | 2.016 | 0.060719991 | |
| OH | 17.008 | 0.041122173 | |
| H_2O | 18.016 | 0.88616989 | |

TABLE IV

Sample Input - Equilibrium Constants*

$$k_c = D_c T^{E_c} e^{F_c/T}$$

| Reaction | DC | EC | FC |
|----------|-------------|--------------|-------------|
| 1 | 0.11519E-01 | 0.33091E-00 | 0.14488E05 |
| 2 | 0.52727E 03 | -0.41176E-00 | -0.15585E05 |
| 3 | 0.15603E 01 | 0.43105E-01 | -0.16202E04 |
| 4 | 0.60708E-02 | 0.18911E-03 | 0.92007E05 |
| 5 | 0.22232E-04 | 0.40971E-00 | 0.10928E06 |
| 6 | 0.64485E-05 | 0.52022E00 | 0.10872E06 |

* Units: lbs moles, ft³, °R

TABLE VI
Output Quantities

| <u>Symbol</u> | <u>Description</u> | <u>Typical Units</u> | <u>Remarks</u> | | |
|----------------|--|--|--------------------------------|---|---|
| X | Axial distance | ft | In print-out for JSUPP = 0,1,2 | | |
| V | Velocity | ft/sec | " | " | " |
| P | Pressure | lb/ft ² | " | " | " |
| DELTAX | The integration step size | ft | In print-out for JSUPP = 0,1,2 | | |
| T | Temperature | °R | " | " | " |
| DT/DX | Temperature slope | °R/ft | " | " | " |
| DP/DX | Pressure slope | lbs/ft ² /ft | In print-out for JSUPP = 0,1,2 | | |
| MF SUM | Sum of the mass fractions | - | " | " | " |
| A | Mach number | - | " | " | " |
| M | Cross-sectional area | ft ² | In print-out for JSUPP = 0,1,2 | | |
| I | Vacuum specific impulse | <u>lb_f-sec</u> <u>lb_m</u> | " | " | " |
| H ₀ | Stagnation enthalpy | <u>BTU</u> <u>lb_m</u> | " | " | " |
| RHO | Density | lb _m /ft ³ | In print-out for JSUPP = 0,1,2 | | |
| DA/DX | Area slope | ft ² /ft | " | " | " |
| GAMMA-P | Process Gamma = $\frac{d \log P}{d \log \rho}$ | - | " | " | " |
| M(DOT) | Mass flow rate | lb _m /sec | In print-out for JSUPP = 0,1,2 | | |

TABLE VI
(Cont.)

| <u>Symbol</u> | <u>Description</u> | <u>Typical Units</u> | <u>Remarks</u> |
|---------------|--|-----------------------------|--------------------------------|
| GAMMA | Frozen Gamma = $\frac{C_P}{C_P - R}$ | - | In print-out for JSUPP = 0,1,2 |
| H | Enthalpy | BTU/lb _m | " " " |
| RAD | Radius assuming nozzle cross section is circular | ft | " " " |
| SIGMA | Concentration | lb-mols/lb _m | In print-out for JSUPP = 0,1 |
| D/DX (SIGMA) | Concentration slope | lb-mols/lb _m -ft | " " " |
| LAMBDA | System 1 = λ | - | In print-out for JSUPP = 0 |
| | System 2 = $\lambda + 1$ | - | " " " |
| D/DX LAMBDA | Slope of λ or $\lambda + 1$ | ft ⁻¹ | " " " |
| PDCTOR | Pn + 1 (see integration) | - | In print-out for JSUPP = 0 |
| CORRECTOR | Cn + 1 (see integration) | - | " " " |

SAMPLE INPUT

* Various forms of E format acceptable.

SAMPLE INPUT, CONT'D

C910096-11

FIG. 2

SAMPLE OUTPUT

| | | | | | | | | | | | |
|---------|---|-------------|--------|---|----------------|----|---|-----------------|---------|---|----------------|
| X | = | 0.28590E-00 | I | = | 2118.19274902 | H | = | 0.41529840E 01 | RHO | = | 0.40311632E-03 |
| V | = | 13850.41150 | DT/DX | = | -0.2096181E 04 | A | = | 0.63528220E-01 | DA/DX | = | 0.73685135E-06 |
| P | = | 107.56006 | DP/DX | = | -0.4981607E 03 | 1 | = | 0.45034252E 03 | GAMMA-P | = | 0.62223411E-03 |
| DELTA X | = | 0.16384E-02 | MF SUM | = | 1.0000010937 | H0 | = | -0.14096821E 04 | M(DOT) | = | 0.23626237E-00 |

SIGMA

| | | |
|-----------------|----------------|-----------------|
| 0.73186267E-06 | LAMBDA | D/DX(SIGMA) |
| 0.622207260E-03 | 0.24323814E-00 | 0.99966382E-06 |
| 0.10433520E-04 | 0.12007992E 02 | -0.32627914E-04 |
| 0.10303967E-01 | 0.26784635E 01 | -0.24076541E-06 |
| 0.97902516E-05 | 0.22484465E 09 | -0.11342777E-04 |
| 0.52052566E-01 | 0.60440374E 09 | -0.52351078E-04 |
| | 0.13755117E 09 | 0.53832273E-04 |

SYSTEM

| | | |
|---|----------------|-----------------|
| 1 | LAMBDA | D/DX(LAMBDA) |
| 1 | 0.24323814E-00 | 0.14236833E 01 |
| 1 | 0.12007992E 02 | -0.30705459E 01 |
| 1 | 0.26784635E 01 | 0.11895368E 02 |
| 1 | 0.22484465E 09 | 0.88227061E 10 |
| 1 | 0.60440374E 09 | 0.25147918E 11 |
| 1 | 0.13755117E 09 | 0.60423587E 10 |

DOCTOR

| | | | | | | | | | | | |
|---------|---|-------------|--------|---|----------------|----|---|-----------------|---------|---|----------------|
| X | = | 0.29082E-00 | I | = | 2108.02020264 | H | = | 0.41664988E 01 | RHO | = | 0.40311632E-03 |
| V | = | 13872.55969 | DT/DX | = | -0.2043357E 04 | A | = | 0.64596558E-01 | DA/DX | = | 0.73685135E-06 |
| P | = | 105.16532 | DP/DX | = | -0.4764359E 03 | 1 | = | 0.45066677E 03 | GAMMA-P | = | 0.62223411E-03 |
| DELTA X | = | 0.16384E-02 | MF SUM | = | 1.000009716 | H0 | = | -0.14096821E 04 | M(DOT) | = | 0.23626237E-00 |

SIGMA

| | | |
|-----------------|----------------|-----------------|
| 0.73186267E-06 | LAMBDA | D/DX(SIGMA) |
| 0.622207260E-03 | 0.24323814E-00 | 0.99966382E-06 |
| 0.10433520E-04 | 0.12007992E 02 | -0.32627914E-04 |
| 0.10303967E-01 | 0.26784635E 01 | -0.24076541E-06 |
| 0.97902516E-05 | 0.22484465E 09 | -0.11342777E-04 |
| 0.52052566E-01 | 0.60440374E 09 | -0.52351078E-04 |
| | 0.13755117E 09 | 0.53832273E-04 |

CORRECTOR

| | | |
|----------------|----------------|-----------------|
| 0.21181927E 04 | LAMBDA | D/DX(LAMBDA) |
| 0.14236833E 01 | 0.24323814E-00 | 0.99966382E-06 |
| 0.30705459E 01 | 0.12007992E 02 | -0.32627914E-04 |
| 0.73184267E-06 | 0.26784635E 01 | -0.24076541E-06 |
| 0.62207260E-03 | 0.22484465E 09 | -0.11342777E-04 |
| 0.24323814E-00 | 0.60440374E 09 | -0.52351078E-04 |
| 0.12007992E 02 | 0.13755117E 09 | 0.53832273E-04 |

SIGMA

| | | |
|-----------------|----------------|-----------------|
| 0.73186267E-06 | LAMBDA | D/DX(SIGMA) |
| 0.622207260E-03 | 0.24323814E-00 | 0.99966382E-06 |
| 0.10433520E-04 | 0.12007992E 02 | -0.32627914E-04 |
| 0.10354763E-04 | 0.26784635E 01 | -0.24076541E-06 |
| 0.50044663E-04 | 0.22484465E 09 | -0.11342777E-04 |
| 0.51465240E-04 | 0.60440374E 09 | -0.52351078E-04 |
| | 0.13755117E 09 | 0.53832273E-04 |

SYSTEM

| | | |
|---|----------------|-----------------|
| 1 | LAMBDA | D/DX(LAMBDA) |
| 1 | 0.25025623E-00 | 0.14318340E 01 |
| 1 | 0.11991803E 02 | -0.35110834E 01 |
| 1 | 0.27369674E 01 | 0.11909440E 02 |
| 1 | 0.27227417E 09 | 0.10521623E 11 |
| 1 | 0.74043566E 09 | 0.30352934E 11 |

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NASA CR-54042
UACRL C910096-11

NAS 3-2572

N64-31452
6/5/65

May 3, 1965

SUPPLEMENT AND ERRATA

→ Investigation of Nonequilibrium Flow Effects

in High Expansion Ratio Nozzles

Computer Program Manual

by

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East Hartford, Connecticut

Use of the Computer Program Manual, NASA CR-54042, and experience acquired with the computer deck described in this manual and available as SHARE program number 3238 has uncovered errors in transcription of several numbers in the sample input listed on page 63 of the Computer Program Manual, and a need for clarification of several items is indicated. This supplement includes new sample input format sheets, Figs. 1 and 2, along with a complete listing of the sample input data, Figs. 3 and 4. The corresponding output, selected to illustrate typical results and operations performed during the machine calculations is also shown in Figs. 5 and 6.

A brief listing and description of the changes to correct and/or clarify the Computer Program Manual and facilitate use of the computer deck are presented below:

1. The computer deck available from SHARE LIBRARY has an undefined branch statement number originating at NECM 1650 in Subroutine Input. This statement should be numbered "10" instead of "4353" in order to complete the compilation and assembly.
2. On page 16, add the following statement to the description of Card 8: "If it is desired to start from the initial value in an area table FFALSE should be set to 0.0 and the table should start at X = 0.0."

NASA CR-54042
UACRL C910096-11

3. On page 18 of the Computer Program Manual, delete the following statement from the description of Card 15: "NOZLNO is the number of nozzles to be calculated from a set of input."
4. On page 19, add the following statement to the description of Card 18: "Each specific heat table must be preceded by the indicator NCPI."
5. The IBM Fortran Format for Card number 15 of Table I, page 54, should read 3I3, 3X, 4I3, 2E6.0.
6. On page 55, delete from Card number 15 under Columns Used, 10-12; under Description, NOZLNO; under Nomenclature, number of nozzles.

SAMPLE INPUT

SAMPLE INPUT, CONT'D

INPUT LISTING

INPUT LISTING (CON'T)

30 540.0+00 6.894+00 720.0+00 6.975+00 900.0+00 6.993+00CP 6
 1080.0+00 7.009+00 1260.0+00 7.036+00 1440.0+00 7.087+00CP 6
 1620.0+00 7.148+00 1800.0+00 7.219+00 1980.0+00 7.304+00CP 6
 2160.0+00 7.390+00 2340.0+00 7.490+00 2520.0+00 7.600+00CP 6
 2700.0+00 7.720+00 2880.0+00 7.823+00 3060.0+00 7.921+00CP 6
 3240.0+00 8.016+00 3422.0+00 8.108+00 3600.0+00 8.195+00CP 6
 3780.0+00 8.279+00 3961.0+00 8.358+00 4140.0+00 8.434+00CP 6
 4320.0+00 8.506+00 4505.0+00 8.575+00 4680.0+00 8.639+00CP 6
 4860.0+00 8.704+00 5040.0+00 8.757+00 5220.0+00 8.810+00CP 6
 5400.0+00 8.859+00 5580.0+00 8.911+00 5760.0+00 8.962+00CP 6

30 540.0+00 7.134+00 720.0+00 7.077+00 900.0+00 7.049+00CP 8
 1080.0+00 7.053+00 1260.0+00 7.087+00 1440.0+00 7.148+00CP 8
 1620.0+00 7.232+00 1800.0+00 7.329+00 1980.0+00 7.436+00CP 8
 2160.0+00 7.548+00 2340.0+00 7.657+00 2520.0+00 7.764+00CP 8
 2700.0+00 7.866+00 2880.0+00 7.963+00 3060.0+00 8.052+00CP 8
 3240.0+00 8.139+00 3422.0+00 8.213+00 3600.0+00 8.285+00CP 8
 3780.0+00 8.352+00 3961.0+00 8.414+00 4140.0+00 8.470+00CP 8
 4320.0+00 8.523+00 4505.0+00 8.573+00 4680.0+00 8.621+00CP 8
 4860.0+00 8.664+00 5040.0+00 8.704+00 5220.0+00 8.742+00CP 8
 5400.0+00 8.778+00 5580.0+00 8.811+00 5760.0+00 8.843+00CP 8

30 540.0+00 8.027+00 720.0+00 8.186+00 900.0+00 8.415+00CP 9
 1080.0+00 8.676+00 1260.0+00 8.954+00 1440.0+00 9.246+00CP 9
 1620.0+00 9.541+00 1800.0+00 9.851+00 1980.0+00 10.152+00CP 9
 2160.0+00 10.444+00 2340.0+00 10.723+00 2520.0+00 10.987+00CP 9
 2700.0+00 11.233+00 2880.0+00 11.462+00 3060.0+00 11.674+00CP 9
 3240.0+00 11.889+00 3422.0+00 12.048+00 3600.0+00 12.214+00CP 9
 3780.0+00 12.366+00 3961.0+00 12.505+00 4140.0+00 12.634+00CP 9
 4320.0+00 12.754+00 4505.0+00 12.863+00 4680.0+00 12.985+00CP 9
 4860.0+00 13.054+00 5040.0+00 13.146+00 5220.0+00 13.228+00CP 9
 5400.0+00 13.304+00 5580.0+00 13.374+00 5760.0+00 13.441+00CP 9

22

*032479231 *012615523
 *034777601 *0115806
 *041552227 *009387
 *04474412 *0091992339
 *047509120 *0092280479
 *07177735 *0111112
 *081777351 *0125128
 *091777351 *0139977
 *101777351 *0139977
 *11177735 *0155659
 *12177735 *0172172
 *16177735 *0267226
 *20177735 *0358184
 *24177735 *0462518
 *32177735 *071113899
 *40177735 *10130309
 *58177735 *1887061
 *88177735 *3943078
 1.08177735 *5729936
 1.58177735 *1.1653712
 2.08177735 *9658390
 3.58177735 *6157834

SAMPLE OUTPUT

C910096-11

FIG. 5

```

0.50933129E 00          0.50933048E 00
0.60870183E 00          0.60870548E 00
0.58086586E 00          0.58086590E 00

X = 0.43776E-01   T = 5183.5509332 IN AT X = 0.44390357E-01 *-*-*-
Y = 4628.81403   DT/DX = 0.88975973E 00 RHO = 0.7850769E-02 GAMMA = 0.1217274E 01
P = 5425.16089   DP/DX = -0.1070438E 05 A = 0.92134029E-02 DA/DX = -0.2724218E-01 H = -0.1837832E 04
DELTAX = 0.12800E-04 MF SUM = 0.999998979 HO = 0.25316568E 03 GAMMA-P = 0.1157683E 01 RADIUS = 0.5415457E-01
                                         M(DOT) = 0.3348127E-00

SIGMA          D/DX(SIGMA)
0.19392607E-03          -0.22642077E-02
0.43123250E-02          -0.17348364E-01
0.13216104E-03          -0.11321381E-02
0.17815807E-02          -0.5430501E-02
0.30000950E-01          -0.1914996E-01
0.22226328E-02          0.23677680E-01
0.49402517E-01

SYSTEM          D/DX(LAMBDA)
1               0.16467075E-00
1               0.23829449E 01
1               0.47851299E-01
1               0.2133092E 02
1               0.24002808E 02
1               0.20231063E 02

LAMBDA          CORRECTOR
0.76686869E-04          0.51835509E 04
0.18750412E-01          0.78507687E-02
0.17815807E-02          0.19392607E-03
0.51282257E 00          0.43123250E-02
0.61263551E 00          0.77830824E-04
0.58424213E 00          0.18749382E-01
0.17812251E-02          0.17812251E-02
0.51282151E 00          0.17816093E-02
0.61263622E 00          0.51282266E 00
0.58424226E 00          0.61263545E 00
                                         RHO = 0.7834150E-02 GAMMA = 0.1217276E 01
                                         DA/DX = -0.2483869E-01 H = -0.1838953E 04
                                         GAMMA-P = 0.1154516E 01 RADIUS = 0.5414867E-01
                                         M(DOT) = 0.3348111E-00

SIGMA          D/DX(LAMBDA)
0.19375267E-03          -0.22510350E-02
0.43109674E-02          -0.1797404E-01
0.13207372E-03          -0.11390807E-02
0.30000542E-01          -0.47591767E-02
0.22211894E-02          -0.18434165E-01
0.49404249E-01          0.22963361E-01

SYSTEM          CORRECTOR
1               0.16168856E 02
1               0.51827639E 04
1               0.78421711E-02

```

SAMPLE OUTPUT

```

1          0.17342438E-02
1          0.53967354E 00
1          0.65039160E 00
1          0.61503769E 00

CORRECTOR
0.51213825E 04
0.70671628E-02
0.17311649E-03
0.41152512E-02
0.50128233E-04
0.22775300E-01
0.17347817E-02
0.53967489E 00
0.65039033E 00
0.61503763E 00
0.173488714600 M = 0.10014168E 01
0.6052965E 04 A = 0.9167176E-02
0.4982590E 05 I = 0.29242948E 03
MF SUM = 1.000002220 H0 = -0.14099725E 04
RHO = 0.70615152E-02
DA/DX = 0.4755168E-02
GAMMA-P = 0.1150557E 01
M(DOT) = 0.3348118E-00
GAMMA = 0.1217209E 01
H = -0.1944084E 04
RADIUS = 0.5401925E-01

SIGMA
0.17299759E-03
0.41141800E-02
0.11913797E-03
0.29975568E-01
0.20675872E-02
0.49604712E-01
D/DX(SIGMA)
-0.14499910E-02
-0.1307035E-01
-0.92200479E-03
-0.26621394E-02
-0.118003313E-01
0.15102313E-01

LAMBDA
0.51301806E-04
0.22781604E-01
0.17345301E-02
0.54042487E 00
0.65127052E 00
0.61588764E 00
D/DX(LAMBDA)
0.25998006E-01
0.672812213E-01
-0.684466265E-02
0.91887411E 01
0.10801058E 02
0.10421829E 02
CORRECTOR
0.51208871E 04
0.70619519E-02
0.17299758E-03
0.41141774E-02
0.53406160E-04
0.22779702E-01
0.17338359E-02
0.54042314E 00
0.65127215E 00
0.61588772E 00
D/DX(LAMBDA)
0.25998006E-01
0.672812213E-01
-0.684466265E-02
0.91887411E 01
0.10801058E 02
0.10421829E 02
***** RUNGE KUTTA RESTART X = 0.56237908E-01 DELTA X = 0.10240000E-04 *****
***** RETURN TO DE SYSTEM 1 FAILED AT X = 0.56647504E-01 *****
X = 0.55787E-01 T = 5120.39086914 M = 0.10021683E 01 RHO = 0.7056742E-02 GAMMA = 0.1217209E 01
Y = 5175.24438 DT/DX = -0.6062472E 04 A = 0.9167106E-02 DA/DX = 0.4867300E-02 H = -0.1944884E 04
P = 4805.23017 DP/DX = -0.4781360E 05 I = 0.29243518E 03 GAMMA-P = 0.1150465E 01 RADIUS = 0.5402041E-01
DELTAX = 0.20480E-04 MF SUM = 1.000002533 H0 = -0.14099733E 04 M(DOT) = 0.3348118E-00
SIGMA
0.17287894E-03
0.41131119E-02
0.11906251E-03
0.29975354E-01
D/DX(SIGMA)
-0.14467546E-02
-0.1298992E-01
-0.91988225E-03
-0.27148053E-02

```